

2-355  
**ONLINE SEARCH REQUEST FORM**

\*\*\*\*\*  
USER DATWU

SERIAL NUMBER 2414863

ART UNIT 122

PHONE X4710

DATE 3/21/95

Please give a detailed statement of requirements. Describe as specifically as possible the subject matter to be searched. Define any terms that may have special meaning. Give examples or relevant citations, authors, or keywords, if known.

You may include a copy of the broadest and/or relevant claim(s).

$\text{Z}-\text{R}-\text{A}-\text{R}'-\text{Y}$

$\text{Z}, \text{Y} =$  cyclic polyamine having 9-20 ring members + 3-6 N atoms

$\text{R}, \text{R}' = -\text{C}-$

A = aromatic or heterocromatic group

Off. rec:

$\text{N}-\text{R}-\text{A}-\text{R}'-\text{N}$

cyclic atoms  
in 9-20 member rings

Bridg. Gary

\*\*\*\*\*  
**STAFF USE ONLY**

COMPLETED

3-25-95

SEARCHER

JIMI DANTZ

ONLINE TIME

60

(in minutes)

TOTAL TIME 82

SYSTEMS

CAS ONLINE

DARC/QUESTEL

DIALOG

SDC

OTHER

=>  
=> d his 17-

(FILE 'CA' ENTERED AT 13:36:51 ON 25 MAR 95)

L7 37 S BRIDGER G?/AU  
L8 2 S L7 AND (HIV OR AIDS OR HTLV OR IMMUNODEFIC)  
L9 1 S L7 AND CYCLIC  
L10 2 S L8 OR L9

=> d all

L10 ANSWER 1 OF 2 CA COPYRIGHT 1995 ACS  
AN 120:30786 CA  
TI Linked heterocyclic polyamines with activity against HIV  
IN Bridger, Gary James; Padmanabhan, Sreenivasan; Skerlj,  
Renato Tony; Thornton, David Michael  
PA Johnson Matthey P.L.C., UK  
SO PCT Int. Appl., 66 pp.  
CODEN: PIXXD2  
PI WO 9312096 A1 930624  
DS W: AU, CA, CS, FI, HU, JP, KR, NO, NZ, PL, RU, US  
RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE  
AI WO 92-GB2334 921216  
PRAI GB 91-26677 911216  
DT Patent  
LA English  
IC ICM C07D257-02  
ICS C07D255-02; C07D259-00; C07D401-14; C07D409-14  
CC 28-23 (Heterocyclic Compounds (More Than One Hetero Atom))  
Section cross-reference(s): 1  
OS MARPAT 120:30786  
AB The title compds. ZRAR1Y [A = arom. or heteroarom. moiety; R, R1 =  
(un)substituted alk. chain or heteroatom-contg. chain; Y, Z =  
cyclic polyamine moieties having 9-32 ring members and 3-8 N  
atoms in the ring spaced by .gtoreq.2 C atoms from each other] or  
their acid addn. salts or metal complexes are prep'd. and  
demonstrated viricidal activity against HIV-1 and  
HIV-2. Thus, 1,1'-(1,4-phenylenebis(methylene))bis-1,4,8,11-  
tetraazacyclotetradecane was prep'd. and demonstrated 50% inhibitory  
concn. against HIV-1 of 0.006 .mu.g/mL and 50% inhibitory  
concn. against HIV-2 of <0.01 .mu.g/mL in an assay  
employing infected MT-4 cells.  
ST AIDS treatment prep'n heterocyclic polyamine; HIV  
virucide prep'n heterocyclic polyamine; tetraazacyclotetradecane  
prep'n HIV viricidal agent; virustat prep'n  
tetraazacyclotetradecane  
IT Virucides and Virustats  
(heterocyclic polyamines)  
IT Virus, animal  
(human immunodeficiency 1, inhibition of, heterocyclic  
polyamines for)  
IT Virus, animal  
(human immunodeficiency 2, inhibition of, heterocyclic  
polyamines for)  
IT 151191-32-1 151191-33-2 151191-34-3 151191-35-4 151191-36-5  
(HIV viricidal activity of)  
IT 7440-50-8DP, Copper, 1,4-phenylenebismethylene bis

tetraazacyclotetradecane complexes 7440-66-6DP, Zinc,  
 1,4-phenylenebisethylene bis tetraazacyclotetradecane complexes

110078-44-9P	110078-46-1DP,	copper and zinc complexes	
133587-10-7P	133587-11-8P	151190-72-6P	151190-73-7P
151190-74-8P	151190-75-9P	151190-76-0P	151190-80-6P
151190-81-7P	151190-85-1P	151190-87-3P	151190-91-9P
151190-93-1P	151190-94-2P	151190-95-3P	151190-96-4P
151190-97-5P	151190-98-6P	151190-99-7P	151191-02-5P
151191-03-6P	151191-05-8P	151191-06-9P	151191-08-1P
151191-09-2P	151191-12-7P	151191-14-9P	151191-15-0P
151191-17-2P	151191-18-3P	151191-20-7P	151191-21-8P
151191-24-1P	151191-25-2P	151191-26-3P	151191-27-4P
151191-28-5P	151191-29-6P	151191-30-9P	151191-31-0P
151191-37-6P	151191-38-7P	151191-39-8P	

(prepn. and HIV viricidal activity of)

IT 19417-58-4P, 1,4-Benzenedipropanol 58791-49-4P 60023-32-7P

63134-93-0P	70364-29-3P	92339-07-6P	105355-16-6P
145617-64-7P	151190-69-1P	151190-70-4P	151190-71-5P
151190-77-1P	151190-79-3P	151190-82-8P	151190-83-9P
151190-84-0P	151190-86-2P	151190-88-4P	151190-89-5P
151190-92-0P	151191-00-3P	151191-01-4P	151191-04-7P
151191-07-0P	151191-10-5P	151191-11-6P	151191-13-8P
151191-16-1P	151191-19-4P	151191-22-9P	

(prepn. and reaction of, in prepn. of heterocyclic HIV  
 viricidal agents)

IT 575-41-7, 1,3-Dimethylnaphthalene 623-24-5, .alpha.,.alpha.'-  
 Dibromo-p-xylene 623-27-8, 1,4-Benzenedicarboxaldehyde 626-15-3,  
 .alpha.,.alpha.'-Dibromo-m-xylene 652-36-8 1099-45-2,  
 Carbethoxymethylene)triphenylphosphorane 1198-37-4,  
 2,4-Dimethylquinoline 4741-99-5, 1,4,8,11-Tetraazaundecane  
 7703-74-4 14647-60-0 24656-53-9 28569-48-4 35991-75-4  
 39568-89-3 66977-70-6 71176-55-1 78831-37-5 94530-07-1  
 104395-69-9 110078-46-1 134457-14-0 151190-78-2 151191-23-0

(reaction of, in prepn. of heterocyclic HIV viricidal  
 agents)

=> fil reg ;d 151190-77-1

FILE 'REGISTRY' ENTERED AT 13:39:08 ON 25 MAR 95

USE IS SUBJECT TO THE TERMS OF YOUR CUSTOMER AGREEMENT

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STRUCTURE FILE UPDATES: 24 MAR 95 HIGHEST RN 161753-30-6

DICTIONARY FILE UPDATES: 24 MAR 95 HIGHEST RN 161753-30-6

TSCA INFORMATION NOW CURRENT THROUGH MAY 1994

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ANSWER 1 REGISTRY COPYRIGHT 1995 ACS

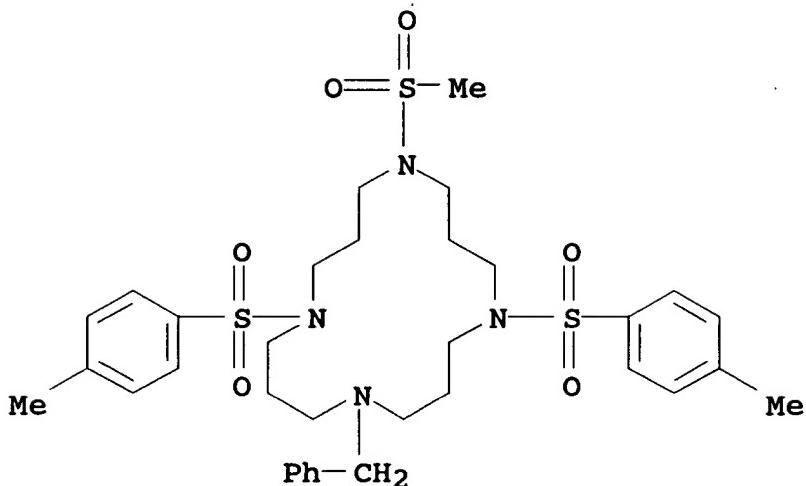
RN 151190-77-1 REGISTRY

CN 1,5,9,13-Tetraazacyclohexadecane, 1,9-bis[(4-methylphenyl)sulfonyl]-  
 5-(methylsulfonyl)-13-(phenylmethyl)-(9CI) (CA INDEX NAME)

FS 3D CONCORD

MF C34 H48 N4 O6 S3

SR CA  
 LC STN Files: CA



1 REFERENCES IN FILE CA (1967 TO DATE)

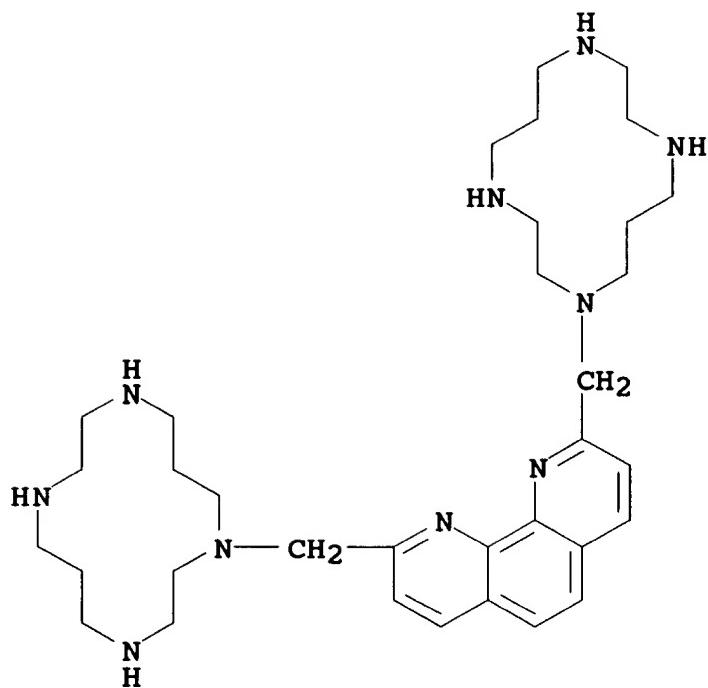
=> fil reg ;d 151190-94-2  
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 DICTIONARY FILE UPDATES: 24 MAR 95 HIGHEST RN 161753-30-6

TSCA INFORMATION NOW CURRENT THROUGH MAY 1994

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ANSWER 1 REGISTRY COPYRIGHT 1995 ACS  
 RN 151190-94-2 REGISTRY  
 CN 1,4,8,11-Tetraazacyclotetradecane, 1,1'-(1,10-phenanthroline-2,9-diylbismethylene)bis- (9CI) (CA INDEX NAME)  
 FS 3D CONCORD  
 MF C34 H56 N10  
 CI COM  
 SR CA  
 LC STN Files: CA



1 REFERENCES IN FILE CA (1967 TO DATE)

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=>

=> fil ca

FILE 'CA' ENTERED AT 13:40:04 ON 25 MAR 95  
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FILE COVERS 1967 - 18 Mar 1995 (950318/ED) VOL 122 ISS 12

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=> d 110 all

L10 ANSWER 1 OF 2 CA COPYRIGHT 1995 ACS  
AN 120:30786 CA  
TI Linked heterocyclic polyamines with activity against HIV  
IN Bridger, Gary James; Padmanabhan, Sreenivasan; Skerlj,  
Renato Tony; Thornton, David Michael  
PA Johnson Matthey P.L.C., UK  
SO PCT Int. Appl., 66 pp.  
CODEN: PIXXD2  
PI WO 9312096 A1 930624  
DS W: AU, CA, CS, FI, HU, JP, KR, NO, NZ, PL, RU, US  
RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE  
AI WO 92-GB2334 921216  
PRAI GB 91-26677 911216  
DT Patent  
LA English  
IC ICM C07D257-02  
ICS C07D255-02; C07D259-00; C07D401-14; C07D409-14  
CC 28-23 (Heterocyclic Compounds (More Than One Hetero Atom))  
Section cross-reference(s): 1  
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AB The title compds. ZRAR1Y [A = arom. or heteroarom. moiety; R, R1 =  
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cyclic polyamine moieties having 9-32 ring members and 3-8 N  
atoms in the ring spaced by .gtoreq.2 C atoms from each other] or  
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concn. against HIV-2 of <0.01 .mu.g/mL in an assay  
employing infected MT-4 cells.  
ST AIDS treatment prepn heterocyclic polyamine; HIV  
virucide prepn heterocyclic polyamine; tetraazacyclotetradecane  
prepn HIV viricidal agent; virustat prepn  
tetraazacyclotetradecane  
IT Viricides and Virustats  
(heterocyclic polyamines)  
IT Virus, animal  
(human immunodeficiency 1, inhibition of, heterocyclic  
polyamines for)

IT Virus, animal  
(human immunodeficiency 2, inhibition of, heterocyclic polyamines for)

IT 151191-32-1 151191-33-2 151191-34-3 151191-35-4 151191-36-5  
(HIV viricidal activity of)

IT 7440-50-8DP, Copper, 1,4-phenylenebismethylene bis tetraazacyclotetradecane complexes 7440-66-6DP, Zinc, 1,4-phenylenebismethylene bis tetraazacyclotetradecane complexes  
110078-44-9P 110078-46-1DP, copper and zinc complexes  
133587-10-7P 133587-11-8P 151190-72-6P 151190-73-7P  
151190-74-8P 151190-75-9P 151190-76-0P 151190-80-6P  
151190-81-7P 151190-85-1P 151190-87-3P 151190-91-9P  
151190-93-1P 151190-94-2P 151190-95-3P 151190-96-4P  
151190-97-5P 151190-98-6P 151190-99-7P 151191-02-5P  
151191-03-6P 151191-05-8P 151191-06-9P 151191-08-1P  
151191-09-2P 151191-12-7P 151191-14-9P 151191-15-0P  
151191-17-2P 151191-18-3P 151191-20-7P 151191-21-8P  
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151191-28-5P 151191-29-6P 151191-30-9P 151191-31-0P  
151191-37-6P 151191-38-7P 151191-39-8P  
(prepn. and HIV viricidal activity of)

IT 19417-58-4P, 1,4-Benzenedipropanol 58791-49-4P 60023-32-7P  
63134-93-0P 70364-29-3P 92339-07-6P 105355-16-6P  
145617-64-7P 151190-69-1P 151190-70-4P 151190-71-5P  
151190-77-1P 151190-79-3P 151190-82-8P 151190-83-9P  
151190-84-0P 151190-86-2P 151190-88-4P 151190-89-5P  
151190-92-0P 151191-00-3P 151191-01-4P 151191-04-7P  
151191-07-0P 151191-10-5P 151191-11-6P 151191-13-8P  
151191-16-1P 151191-19-4P 151191-22-9P  
(prepn. and reaction of, in prepn. of heterocyclic HIV viricidal agents)

IT 575-41-7, 1,3-Dimethylnaphthalene 623-24-5, .alpha.,.alpha.'-Dibromo-p-xylene 623-27-8, 1,4-Benzenedicarboxaldehyde 626-15-3, .alpha.,.alpha.'-Dibromo-m-xylene 652-36-8 1099-45-2, Carbethoxymethylene)triphenylphosphorane 1198-37-4, 2,4-Dimethylquinoline 4741-99-5, 1,4,8,11-Tetraazaundecane 7703-74-4 14647-60-0 24656-53-9 28569-48-4 35991-75-4 39568-89-3 66977-70-6 71176-55-1 78831-37-5 94530-07-1 104395-69-9 110078-46-1 134457-14-0 151190-78-2 151191-23-0  
(reaction of, in prepn. of heterocyclic HIV viricidal agents)

=> d 110 all 2

L10 ANSWER 2 OF 2 CA COPYRIGHT 1995 ACS  
AN 118:80485 CA  
TI Preparation of polyaza(cyclo)alkanes as antiviral compounds  
IN Schwartz, David Aaron; Bridger, Gary  
PA Johnson Matthey PLC, UK  
SO PCT Int. Appl., 26 pp.  
CODEN: PIXXD2  
PI WO 9216494 A1 921001  
DS W: AU, CA, FI, HU, JP, KR, NO, US  
RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LU, MC, NL, SE  
AI WO 92-GB438 920311  
PRAI GB 91-5489 910315  
DT Patent  
LA English  
IC ICM C07C211-14  
ICS C07D257-02; A61K031-13; A61K031-395  
CC 23-4 (Aliphatic Compounds)  
Section cross-reference(s): 28  
OS MARPAT 118:80485  
AB Title compds. Z(A)nY (Z, Y = 9 to 32-membered poly(hetero)alkyl chain, -poly(hetero)cycloalkyl moiety, each Z, Y having 3-8 heteroatoms selected from N, O, S such that at least 1 of Z, Y is the above chain; A = linking atom or group; n = 0-6), their salts metal complexes, are prepd. against HIV in std. tests. H<sub>2</sub>N(CH<sub>2</sub>)CO<sub>2</sub>H was xl-tosylated, the product esterified with N-hydroxysuccinimide, the ester treated with 1,2,3,4-meso-tetraaminobutane, the tetraamido-tetratosylate treated with borane. THF complex and the product in HBR/AcOH was heated at 100.degree. for 48 h to give meso-1,2,3,4-tetrakis(N-1,3-diaminopropyl)butane (I). In a std. in vitro test I against both HIV-1 and HIV-1 had a selectivity index (ratio of CD50 and ED50) of >13 compared with AZT >125.  
ST tetrakisdiaminopropylbutate prepn virucide HIV;  
tetraazacyclotetradecylbenzomethyl bis prepn virucide HIV  
IT Virus, animal  
(human immunodeficiency 1, infection with, treatment  
of, tetrakis(diaminopropyl)butane and  
tetraazacyclotetradecylbenzenemethylbis for)  
IT Virus, animal  
(human immunodeficiency 2, infection with, treatment  
of, tetrakis(diaminopropyl)butane and  
tetraazacyclotetradecylbenzenemethylbis for)  
IT 42908-33-8P 145617-61-4P 145617-62-5P 145617-63-6P  
145617-64-7P 145617-65-8P 145617-66-9P 145617-67-0P  
145617-68-1P 145617-69-2P  
(prepn. and reaction of, in prepn. of HIV virucides)  
IT 145617-56-7P 145617-57-8P 145617-58-9P 145617-59-0P  
145617-60-3P  
(prepn. of, as HIV virucide)  
IT 107-95-9, 3-Aminopropanoic acid 112-24-3 623-24-5 10563-26-5,  
N,N'-Bis(3-aminopropyl)ethylenediamine 74676-47-4 92902-03-9  
104395-69-9  
(reaction of, in prepn. of HIV virucides)

=>

=> fil reg;d 145617-64-7

FILE 'REGISTRY' ENTERED AT 13:40:40 ON 25 MAR 95

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DICTIONARY FILE UPDATES: 24 MAR 95 HIGHEST RN 161753-30-6

TSCA INFORMATION NOW CURRENT THROUGH MAY 1994

Please note that search-term pricing does apply when  
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ANSWER 1 REGISTRY COPYRIGHT 1995 ACS

RN 145617-64-7 REGISTRY

CN 1,4,8,11-Tetraazacyclotetradecane, 1-[[4-(bromomethyl)phenyl]methyl]-  
4,8,11-tris[(4-methylphenyl)sulfonyl]- (9CI) (CA INDEX NAME)

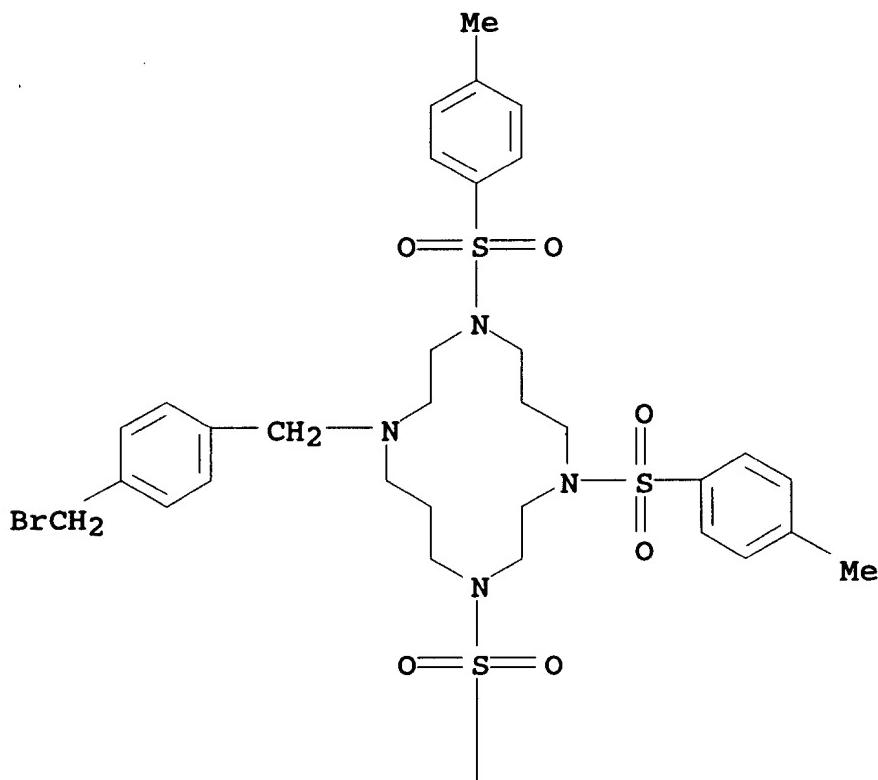
FS 3D CONCORD

MF C39 H49 Br N4 O6 S3

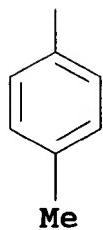
SR CA

LC STN Files: CA

PAGE 1-A



PAGE 2-A



2 REFERENCES IN FILE CA (1967 TO DATE)

=> fil reg

FILE 'REGISTRY' ENTERED AT 14:07:02 ON 25 MAR 95  
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=> d que 128

L11 STR

N 1 N 3 N 5

NODE ATTRIBUTES:

NSPEC IS R AT 1  
NSPEC IS R AT 3  
NSPEC IS R AT 5

DEFAULT MLEVEL IS ATOM

DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED  
NUMBER OF NODES IS 3

STEREO ATTRIBUTES: NONE

L13 STR

N—C—Cy—C—N  
1 2 3 4 5

NODE ATTRIBUTES:

NSPEC IS R AT 1  
NSPEC IS R AT 5  
DEFAULT MLEVEL IS ATOM  
GGCAT IS UNS AT 3  
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED  
NUMBER OF NODES IS 5

STEREO ATTRIBUTES: NONE

L17 STR

Hy—C—Cy—C—Hy  
1 2 3 4 5

NODE ATTRIBUTES:

DEFAULT MLEVEL IS ATOM  
GGCAT IS HIQ AT 1

GGCAT IS UNS AT 3  
 GGCAT IS HIQ AT 5  
 DEFAULT ECLEVEL IS LIMITED  
 ECOUNT IS M4 C M3 N AT 1  
 ECOUNT IS M4 C M3 N AT 5

## GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED  
 NUMBER OF NODES IS 5

STEREO ATTRIBUTES: NONE  
 L19 STR



## NODE ATTRIBUTES:

DEFAULT MLEVEL IS ATOM  
 DEFAULT ECLEVEL IS LIMITED

## GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED  
 NUMBER OF NODES IS 10

STEREO ATTRIBUTES: NONE

L22 SCR 1840 AND 1996 AND 140 AND 1607 AND 1236  
 L23 SCR 1840 AND 1996 AND 140 AND 1607 AND 1363  
 L28 308 SEA FILE=REGISTRY SSS FUL L11 AND L13 AND L17 AND L19 AND  
 (L22 OR L23)

=> fil ca

FILE 'CA' ENTERED AT 14:07:15 ON 25 MAR 95  
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(FILE 'REGISTRY' ENTERED AT 13:40:40 ON 25 MAR 95)  
 L28 308 S L11 AND L13 AND L17 AND L19 AND (L22 OR L23) FUL

FILE 'CA' ENTERED AT 14:05:18 ON 25 MAR 95  
 L29 75 S L28  
 L30 2 S L29(L)(VIRU? OR ANTIVIR? OR AIDS OR HIV OR HTLV OR IMMU  
 L31 2 S L29 AND (VIRU? OR ANTIVIR? OR AIDS OR HIV OR HTLV OR IM

FILE 'REGISTRY' ENTERED AT 14:07:02 ON 25 MAR 95

FILE 'CA' ENTERED AT 14:07:15 ON 25 MAR 95

=> d.all

L31 ANSWER 1 OF 2 CA COPYRIGHT 1995 ACS  
AN 120:289504 CA  
TI Highly potent and selective inhibition of human immunodeficiency virus by the bicyclam derivative JM3100  
AU De Clercq, Erik; Yamamoto, Naohiko; Pauwels, Rudi; Balzarini, Jan; Witvrouw, Myriam; De Vreese, Karen; Debyser, Zeger; Rosenwirth, Brigitte; Peichl, Peter; et al.  
CS Rega Inst. Med. Res., Kathol. Univ. Leuven, Louvain, B-3000, Belg.  
SO Antimicrob. Agents Chemother. (1994), 38(4), 668-74  
CODEN: AMACQ; ISSN: 0066-4804  
DT Journal  
LA English  
CC 1-5 (Pharmacology)  
AB Bicyclams, in which the cyclam (1,4,8,11-tetraazacyclotetradecane) moieties are tethered via an aliph. bridge (i.e., propylene, as in JM2763) are potent and selective inhibitors of human immunodeficiency virus type 1 (HIV-1) and type-2 (HIV-2) (E. De Clercq, N. Yamamoto, R. Pauwels, M. Baba, D. Schols, H. Nakashima, J. Balzarini, Z. Debyser, B. A., Murrer, D. Schwartz, D. Thornton, G. Bridger, S. Fricker, G. Henson, M. Abrams, and D. Picker, Proc. Natl. Acad. Sci. USA 89:5286-5290, 1992). The authors have now found that the bicyclam JM3100, in which the cyclam moieties are tethered by an arom. bridge [i.e., phenylenebis(methylene)], inhibits the replication of various HIV-1 and HIV-2 strains in various cell lines at a 50% effective concn. (EC50) of 1 to 10 ng/mL, which is about 100-fold lower than the concn. required for JM2763 to inhibit HIV replication and at least 100,000-fold lower than the concn. required for JM2763 to inhibit HIV replication and at least 100,000-fold lower than the cytotoxic concn. (>500 .mu.g/mL). In primary T4 lymphocytes or primary monocytes, JM3100 proved inhibitory to HIV-1 (IIIB) and several clin. HIV-1 isolated at an EC50 of less than 1 ng/mL. On the basis of time-of-addn. expts., JM3100 appeared to interact with a viral uncoating event, and this was further corroborated by an uncoating assay in which RNase sensitivity of [5-3H]uridine-labeled virions was monitored. In addn., but possibly mechanistically related, JM3100 blocks formation of infectious particles. JM3100 was also found to interfere directly with virus-induced syncytium formation, albeit at a higher concn. (1 to 2 .mu.g/mL) than that required for inhibition of viral replication. Following s.c. injection of 10 mg of JM3100 per kg of body wt. to rabbits, anti-HIV activity was detected in serum corresponding to serum drug levels exceeding for at least 6 h by >100-fold the EC50 required to inhibit HIV replication in vitro. When combined with either 3'-azido-2',3'-dideoxythymidine or 2',3'-dideoxyinosine, JM3100 achieved a additive inhibition of HIV replication, and when repeatedly subcultivated in the presence of JM3100, the virus remained insensitive to the compd. for at least 30 passages (120 days) in cell culture.  
ST HIV virus inhibition bicyclam deriv JM3100  
IT Virucides and Virustats  
(bicyclam derivs. as, structure in relation to, in human cells)  
IT Drug interactions

(of bicyclam deriv. JM3100 and dideoxynucleosides, in **HIV virus** inhibition in human cells)  
IT Drug resistance  
    (to bicyclam deriv. JM3100, in **HIV virus** in human cells)  
IT **virus, animal**  
    (human **immunodeficiency 1**, inhibition of, by bicyclam deriv. JM3100, in human cells)  
IT **virus, animal**  
    (human **immunodeficiency 2**, inhibition of, by bicyclam deriv. JM3100, in human cells)  
IT Microbicidal and microbiostatic action  
    (virucidal, of bicyclam deriv. JM3100, against **HIV virus** in human cells)  
IT Molecular structure-biological activity relationship  
    (virucidal, of bicyclam derivs., against **HIV virus** in human cells)  
IT 30516-87-1, 3'-Azido-2',3'-dideoxythymidine 69655-05-6,  
2',3'-Dideoxyinosine  
    (**HIV virus** inhibition by, bicyclam deriv. JM3100 enhancement of, in human cells)  
IT 155148-31-5  
    (**HIV virus** inhibition by, mechanism of, structure in relation to, in human cells)  
IT 110078-40-5, JM2763 110078-44-9 151191-06-9  
151191-09-2 155148-32-6  
    (**HIV virus** inhibition by, structure in relation to, in human cells)

=> fil reg

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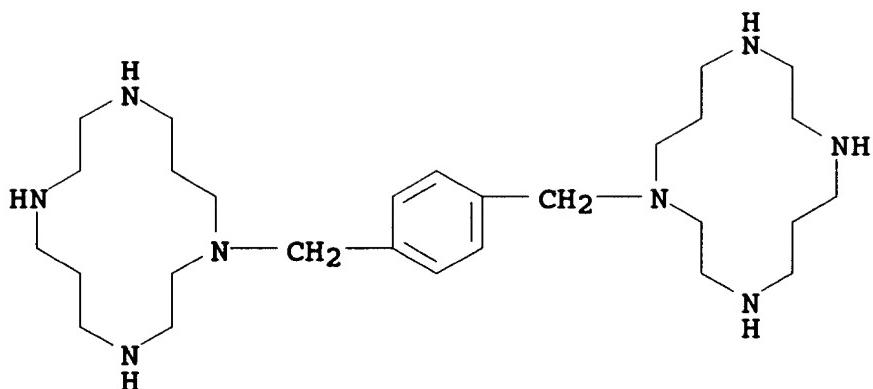
STRUCTURE FILE UPDATES: 24 MAR 95 HIGHEST RN 161753-30-6  
DICTIONARY FILE UPDATES: 24 MAR 95 HIGHEST RN 161753-30-6

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=> d 155148-31-5 110078-44-9

ANSWER 1 REGISTRY COPYRIGHT 1995 ACS  
RN 155148-31-5 REGISTRY  
CN 1,4,8,11-Tetraazacyclotetradecane, 1,1'-[1,4-phenylenebis(methylene)]bis-, octahydrochloride (9CI) (CA INDEX NAME)  
MF C28 H54 N8 . 8 Cl H  
SR CA  
LC STN Files: CA, TOXLIT  
CRN (110078-46-1)



*These compd  
are in above*

● 8 HCl

1 REFERENCES IN FILE CA (1967 TO DATE)

ANSWER 2 REGISTRY COPYRIGHT 1995 ACS

RN 110078-44-9 REGISTRY

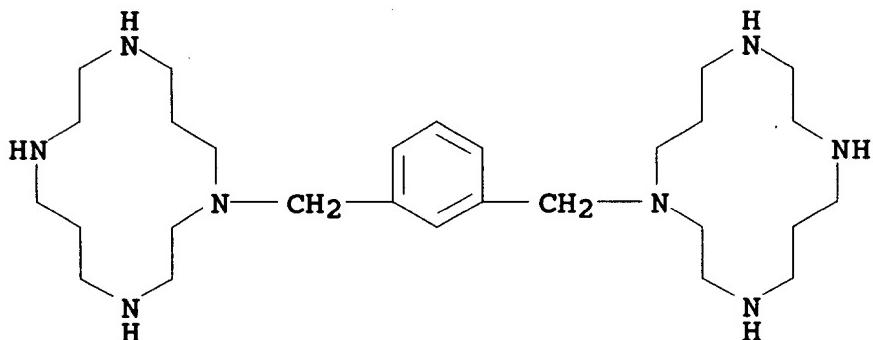
CN 1,4,8,11-Tetraazacyclotetradecane, 1,1'-(1,3-phenylenebis(methylene))bis- (9CI) (CA INDEX NAME)

FS 3D CONCORD

MF C28 H54 N8

SR CA

LC STN Files: BEILSTEIN\*, CA, CHEMINFORMRX, CJACS, TOXLIT, USPATFULL  
(\*File contains numerically searchable property data)



5 REFERENCES IN FILE CA (1967 TO DATE)

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=> d all 2

L31 ANSWER 2 OF 2 CA COPYRIGHT 1995 ACS  
AN 120:30786 CA  
TI Linked heterocyclic polyamines with activity against HIV  
IN Bridger, Gary James; Padmanabhan, Sreenivasan; Skerlj, Renato Tony;  
Thornton, David Michael  
PA Johnson Matthey P.L.C., UK  
SO PCT Int. Appl., 66 pp.  
CODEN: PIXXD2  
PI WO 9312096 A1 930624  
DS W: AU, CA, CS, FI, HU, JP, KR, NO, NZ, PL, RU, US  
RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE  
AI WO 92-GB2334 921216  
PRAI GB 91-26677 911216  
DT Patent  
LA English  
IC ICM C07D257-02  
ICS C07D255-02; C07D259-00; C07D401-14; C07D409-14  
CC 28-23 (Heterocyclic Compounds (More Than One Hetero Atom))  
Section cross-reference(s): 1  
OS MARPAT 120:30786  
AB The title compds. ZRAR1Y [A = arom. or heteroarom. moiety; R, R1 =  
(un)substituted alk. chain or heteroatom-contg. chain; Y, Z = cyclic  
polyamine moieties having 9-32 ring members and 3-8 N atoms in the  
ring spaced by .gtoreq.2 C atoms from each other] or their acid  
addn. salts or metal complexes are prep'd. and demonstrated viricidal  
activity against HIV-1 and HIV-2. Thus,  
1,1'-[1,4-phenylenebis(methylene)]bis-1,4,8,11-  
tetraazacyclotetradecane was prep'd. and demonstrated 50% inhibitory  
concn. against HIV-1 of 0.006 .mu.g/mL and 50% inhibitory  
concn. against HIV-2 of <0.01 .mu.g/mL in an assay  
employing infected MT-4 cells.  
ST AIDS treatment prep heterocyclic polyamine; HIV  
virucide prep heterocyclic polyamine;  
tetraazacyclotetradecane prep HIV viricidal agent;  
virustat prep tetraazacyclotetradecane  
IT Viricides and Virustats  
(heterocyclic polyamines)  
IT Virus, animal  
(human immunodeficiency 1, inhibition of, heterocyclic

polyamines for)

IT virus, animal  
 (human immunodeficiency 2, inhibition of, heterocyclic polyamines for)

IT 151191-32-1 151191-33-2 151191-34-3  
 151191-35-4 151191-36-5  
 (HIV viricidal activity of)

IT 7440-50-8DP, Copper, 1,4-phenylenebismethylene bis tetraazacyclotetradecane complexes 7440-66-6DP, Zinc, 1,4-phenylenebismethylene bis tetraazacyclotetradecane complexes  
 110078-44-9P 110078-46-1DP, copper and zinc complexes 133587-10-7P 133587-11-8P  
 151190-72-6P 151190-73-7P 151190-74-8P  
 151190-75-9P 151190-76-0P 151190-80-6P  
 151190-81-7P 151190-85-1P 151190-87-3P  
 151190-91-9P 151190-93-1P 151190-94-2P  
 151190-95-3P 151190-96-4P 151190-97-5P  
 151190-98-6P 151190-99-7P 151191-02-5P  
 151191-03-6P 151191-05-8P 151191-06-9P  
 151191-08-1P 151191-09-2P 151191-12-7P  
 151191-14-9P 151191-15-0P 151191-17-2P  
 151191-18-3P 151191-20-7P 151191-21-8P  
 151191-24-1P 151191-25-2P 151191-26-3P  
 151191-27-4P 151191-28-5P 151191-29-6P  
 151191-30-9P 151191-31-0P 151191-37-6P  
 151191-38-7P 151191-39-8P  
 (prepn. and HIV viricidal activity of)

IT 19417-58-4P, 1,4-Benzenedipropanol 58791-49-4P 60023-32-7P  
 63134-93-0P 70364-29-3P 92339-07-6P 105355-16-6P  
 145617-64-7P 151190-69-1P 151190-70-4P  
 151190-71-5P 151190-77-1P 151190-79-3P 151190-82-8P  
 151190-83-9P 151190-84-0P 151190-86-2P 151190-88-4P  
 151190-89-5P 151190-92-0P 151191-00-3P  
 151191-01-4P 151191-04-7P 151191-07-0P  
 151191-10-5P 151191-11-6P 151191-13-8P  
 151191-16-1P 151191-19-4P 151191-22-9P  
 (prepn. and reaction of, in prepn. of heterocyclic HIV viricidal agents)

IT 575-41-7, 1,3-Dimethylnaphthalene 623-24-5, .alpha.,.alpha.'-Dibromo-p-xylene 623-27-8, 1,4-Benzenedicarboxaldehyde 626-15-3, .alpha.,.alpha.'-Dibromo-m-xylene 652-36-8 1099-45-2, Carbethoxymethylene)triphenylphosphorane 1198-37-4, 2,4-Dimethylquinoline 4741-99-5, 1,4,8,11-Tetraazaundecane 7703-74-4 14647-60-0 24656-53-9 28569-48-4 35991-75-4 39568-89-3 66977-70-6 71176-55-1 78831-37-5 94530-07-1 104395-69-9 110078-46-1 134457-14-0 151190-78-2  
 151191-23-0  
 (reaction of, in prepn. of heterocyclic HIV viricidal agents)

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=> d 155148-31-5 110078-46-1 151191-07-0
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'110078-46-1' IS NOT A VALID FORMAT FOR FILE 'CA'
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RN 155148-31-5 REGISTRY

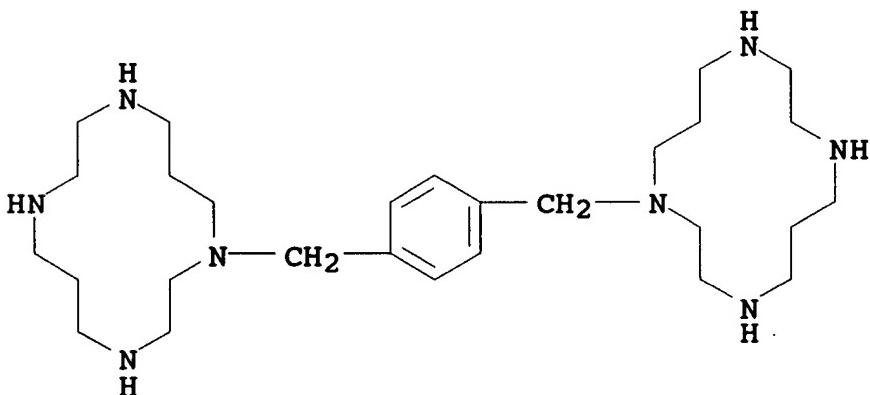
CN 1,4,8,11-Tetraazacyclotetradecane, 1,1'-[1,4-  
 phenylenebis(methylene)]bis-, octahydrochloride (9CI) (CA INDEX  
 NAME)

MF C28 H54 N8 . 8 Cl H

SR CA

LC STN Files: CA, TOXLIT

CRN (110078-46-1)



*These imps  
 are in above*

● 8 HCl

#### 1 REFERENCES IN FILE CA (1967 TO DATE)

ANSWER 2 REGISTRY COPYRIGHT 1995 ACS

RN 110078-46-1 REGISTRY

CN 1,4,8,11-Tetraazacyclotetradecane, 1,1'-[1,4-  
 phenylenebis(methylene)]bis- (9CI) (CA INDEX NAME)

FS 3D CONCORD

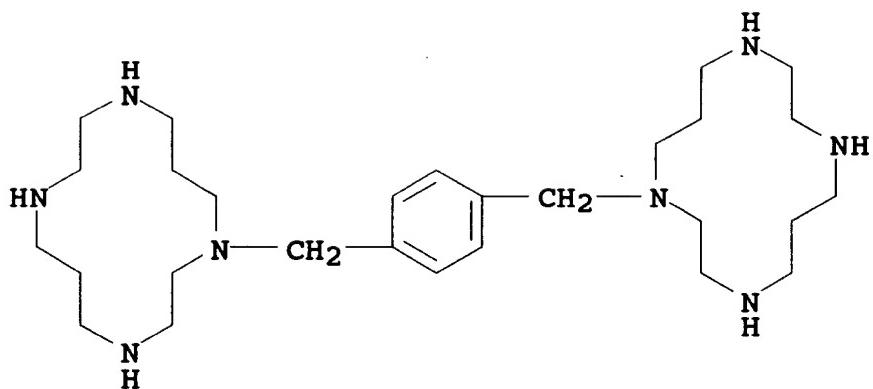
MF C28 H54 N8

CI COM

SR CA

LC STN Files: BEILSTEIN\*, CA, CJACS, USPATFULL

(\*File contains numerically searchable property data)



4 REFERENCES IN FILE CA (1967 TO DATE)

2 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA

ANSWER 3 REGISTRY COPYRIGHT 1995 ACS

RN 151191-07-0 REGISTRY

CN 1,4,8,11-Tetraazacyclotetradecane, 1,1'-[3,5-pyridinediyl]bis(methylene)bis[4,8,11-tris[(4-methylphenyl)sulfonyl]- (9CI) (CA INDEX NAME)

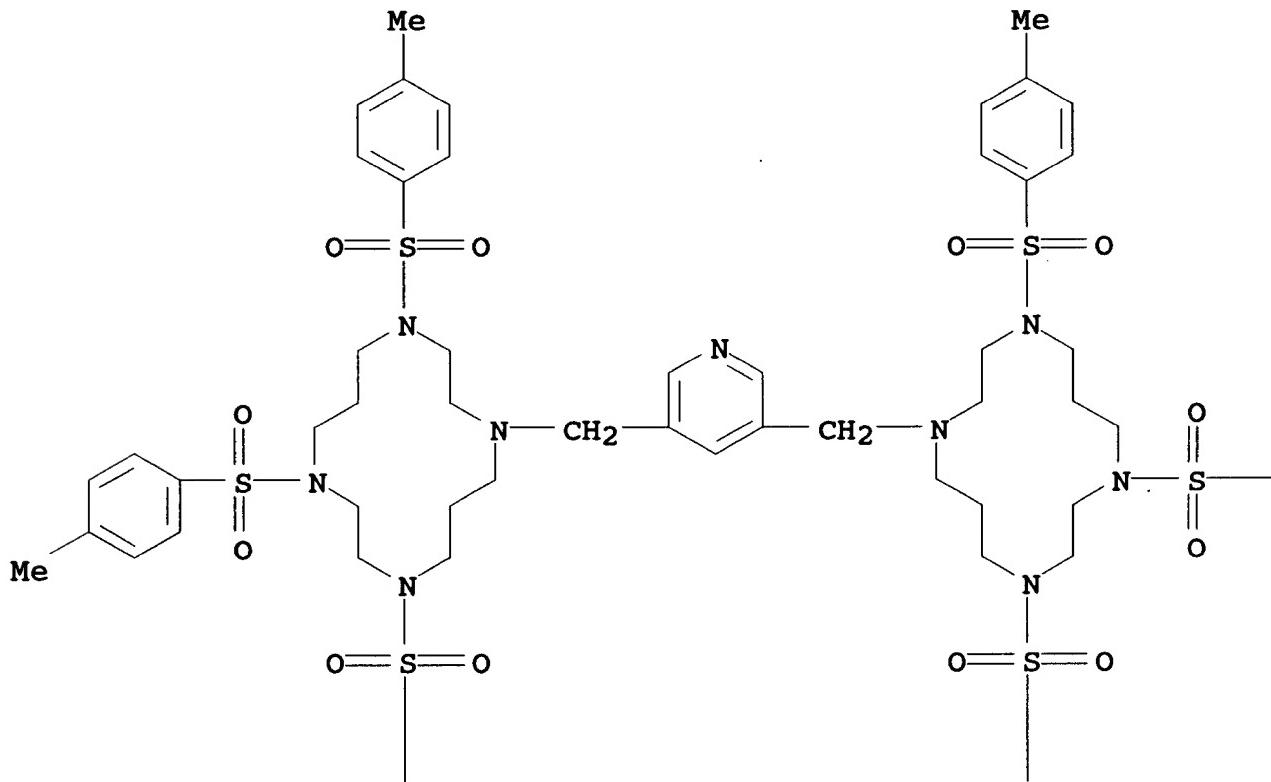
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MF C69 H89 N9 O12 S6

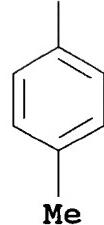
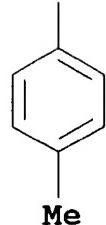
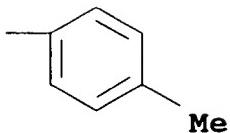
SR CA

LC STN Files: CA

PAGE 1-A



PAGE 1-B



PAGE 2-A

## 1 REFERENCES IN FILE CA (1967 TO DATE)

=&gt; d his

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FILE 'REGISTRY' ENTERED AT 13:28:34 ON 25 MAR 95

L1 STR  
L2 SCR 1847 AND 1996  
L3 50 S L1 AND L2  
L4 STR  
L5 17 S L1 AND L4  
L6 50 S L1 AND L4 AND L2

FILE 'CA' ENTERED AT 13:36:51 ON 25 MAR 95

L7 37 S BRIDGER G?/AU  
L8 2 S L7 AND (HIV OR AIDS OR HTLV OR IMMUNODEFIC?)  
L9 1 S L7 AND CYCLIC  
L10 2 S L8 OR L9

FILE 'REGISTRY' ENTERED AT 13:39:08 ON 25 MAR 95

FILE 'REGISTRY' ENTERED AT 13:39:35 ON 25 MAR 95

FILE 'CA' ENTERED AT 13:40:04 ON 25 MAR 95

FILE 'REGISTRY' ENTERED AT 13:40:40 ON 25 MAR 95

L11 STR L1  
L12 STR L4  
L13 STR L12  
L14 0 S L11 AND L12 AND L13  
L15 SCR 1840 AND 1996  
L16 4 S L11 AND L12 AND L13 AND L15  
L17 STR L12  
L18 3 S L11 AND L13 AND L17 AND L15  
L19 STR  
L20 4 S L11 AND L13 AND L17 AND L19 AND L15  
L21 7 S L11 AND L13 AND L19 AND L15  
L22 SCR 1840 AND 1996 AND 140 AND 1607 AND 1236  
L23 SCR 1840 AND 1996 AND 140 AND 1607 AND 1363  
L24 14 S L11 AND L13 AND L19 AND (L22 OR L23)  
L25 8 S L11 AND L13 AND L17 AND L19 AND (L22 OR L23)  
L26 50 S L1 AND L13 AND L17 AND L19 AND (L22 OR L23)  
L27 50 S L25 OR L26  
L28 308 S L11 AND L13 AND L17 AND L19 AND (L22 OR L23) FUL

FILE 'CA' ENTERED AT 14:05:18 ON 25 MAR 95

L29 75 S L28  
L30 2 S L29(L) (VIRU? OR ANTIVIR? OR AIDS OR HIV OR HTLV OR IMMU  
L31 2 S L29 AND (VIRU? OR ANTIVIR? OR AIDS OR HIV OR HTLV OR IM

FILE 'REGISTRY' ENTERED AT 14:07:02 ON 25 MAR 95

FILE 'CA' ENTERED AT 14:07:15 ON 25 MAR 95

FILE 'REGISTRY' ENTERED AT 14:07:31 ON 25 MAR 95

FILE 'CA' ENTERED AT 14:08:05 ON 25 MAR 95

FILE 'REGISTRY' ENTERED AT 14:08:57 ON 25 MAR 95

FILE 'CA' ENTERED AT 14:09:21 ON 25 MAR 95

L32 4 S L29 AND PHARMAC?/SC,SX  
L33 2 S L32 NOT L31

=>

=>

=> d all

L33 ANSWER 1 OF 2 CA COPYRIGHT 1995 ACS

AN 118:160633 CA

TI Synthesis, DNA binding interactions and biological activity of bis-platinum (II) complexes of N,N,N',N'-tetrakis(2-aminoethyl)diamines

AU Palmer, Brian D.; Wickham, Geoffrey; Craik, David J.; McFadyen, W. David; Wakelin, Laurence P. G.; Baguley, Bruce C.; Denny, William A.

CS Sch. Med., Univ. Auckland, Auckland, N. Z.

SO Anti-Cancer Drug Des. (1992), 7(5), 385-401

DT CODEN: ACDDEA; ISSN: 0266-9536  
LA Journal  
CC English  
CC 1-6 (Pharmacology)  
AB Section cross-reference(s): 23, 25, 78  
AB A series of dimers of the monofunctional platinum species [Pt(dien)Cl]<sup>+</sup>, linked by a variety of flexible (polymethylene) and more rigid chains, was prep'd. and evaluated for DNA interactions and cytotoxic activity. The polymethylene-linked dimers were prep'd. by acylation of N<sub>1</sub>,N<sub>3</sub>-bistrityldiethylenetriamine with .alpha.,.omega.-dicarboxylic acid chlorides, followed by redn. with diborane. Platination of these ligands was achieved with K<sub>2</sub>PtI<sub>4</sub> prep'd. in situ, followed by anion exchange. Solns. of the bis(Pt(dien)Cl)<sub>2</sub><sup>+</sup> complexes were stable, and shown to be pure by <sup>195</sup>Pt NMR, but solid products could not be isolated. All of the bis(Pt(dien)Cl)<sub>2</sub><sup>+</sup> complexes unwound closed circular supercoiled DNA more efficiently than the monomer, and were more efficient than the difunctional platinum complex cisplatin at crosslinking linearized plasmid NDA, as measured on non-denaturing agarose gels. None of the bis(Pt(dien)Cl)<sub>2</sub><sup>+</sup> complexes were as cytotoxic as cisplatin in both the wild-type and platinum-resistant P388 murine leukemia cell lines. The more rigid analogs were equitoxic in both sensitive and cisplatin-resistant cells, but none showed in vitro activity against the P388 tumor.  
ST tetrakisaminoethyldiamine platinum complex antitumor prepn;  
IT aminoethyldiamine platinum complex antitumor prepn  
IT Deoxyribonucleic acids  
IT (bis-platinum tetrakis(aminoethyl)diamine complexes binding of,  
antitumor activity in relation to)  
IT Neoplasm inhibitors  
IT (bis-platinum tetrakis(aminoethyl)diamine complexes, prepn. and  
DNA binding of)  
IT Crosslinking  
IT (of bis-platinum tetrakis(aminoethyl)diamine complexes, by DNA)  
IT Kinetics, reaction  
IT (of platinum tetrakis(aminoethyl)diamine complexes, with DNA,  
antitumor activity in relation to)  
IT 79-37-8, Oxalyl chloride 543-20-4, Succinyl chloride 1663-67-8,  
Malonyl chloride 90421-57-1  
IT (acylation by, of bistrityldiethylenamine)  
IT 100-39-0, Benzyl bromide  
IT (alkylation by, of bistrityldiethylenamine)  
IT 623-24-5 626-15-3 628-77-3, 1,5-Diodopentane  
IT (alkylation by, of bistrityldiethylenetriamine)  
IT 76-83-5, Trityl chloride  
IT (alkylation by, of diethylenetriamine)  
IT 15663-27-1  
IT (antitumor activity and DNA binding interaction of,  
aminoethyldiamine platinum complexes in relation to)  
IT 1877-77-6, 3-(Hydroxymethyl)aniline  
IT (chlorine substitution reaction of)  
IT 10025-99-7  
IT (complexation of, with diamines)  
IT 6232-88-8, 4-(Bromomethyl)benzoic acid  
IT (conversion of, to acid chloride)  
IT 145901-58-2P  
IT (prepn. and alkylation of, with benzyl halides or

haloalkylbenzamide derivs.)  
IT 876-08-4P, 4-(Chloromethyl)benzoyl chloride  
(prepn. and amidation by, of (chloromethyl)aniline)  
IT 145883-50-7P  
(prepn. and amidation of, with (chloromethyl)benzoyl chloride)  
IT 14215-58-8P 18509-61-0P 145901-59-3P 146283-44-5P  
146283-45-6P 146283-46-7P 146283-47-8P  
146283-48-9P 146291-98-7P 146755-38-6P  
(prepn. and antitumor activity of, DNA binding interaction in  
relation to)  
IT 145883-53-0P  
(prepn. and complexation with platinum complexes)  
IT 146735-46-8P  
(prepn. and conversion to chloride complex)  
IT 145883-52-9P 145883-54-1P 145883-59-6P  
(prepn. and detritylation of)  
IT 145883-51-8P  
(prepn. and reaction with bis(trityldiethylenetriamine))  
IT 23539-10-8P 71277-15-1P 73571-38-7P 142745-41-3P  
145883-55-2P 145883-61-0P 145883-62-1P  
(prepn. and reaction with platinum complexes)  
IT 145883-58-5P  
(prepn. and redn. of)  
IT 13528-04-6P 145883-56-3P 145883-57-4P 145883-60-9P  
(prepn. of)  
IT 111-40-0, Diethylenetriamine  
(tritylation of)

=> fil reg;d 146283-46-7 146283-47-8 146291-98-7

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are in  
abundance*

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RN 146283-46-7 REGISTRY

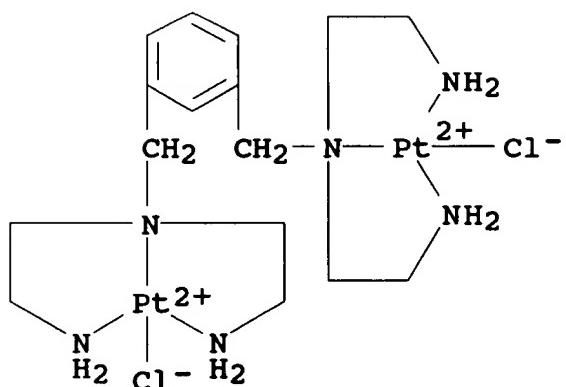
CN Platinum(2+), dichloro[.mu.-[N,N,N',N'-tetrakis(2-aminoethyl)-1,3-benzenedimethanamine-N1,N1',N1'':N3,N3',N3'']]di-, dichloride (9CI)  
(CA INDEX NAME)

MF C16 H32 Cl2 N6 Pt2 . 2 Cl

CI CCS

SR CA

LC STN Files: CA, TOXLIT



● 2 Cl<sup>-</sup>

1 REFERENCES IN FILE CA (1967 TO DATE)

ANSWER 2 REGISTRY COPYRIGHT 1995 ACS

RN 146283-47-8 REGISTRY

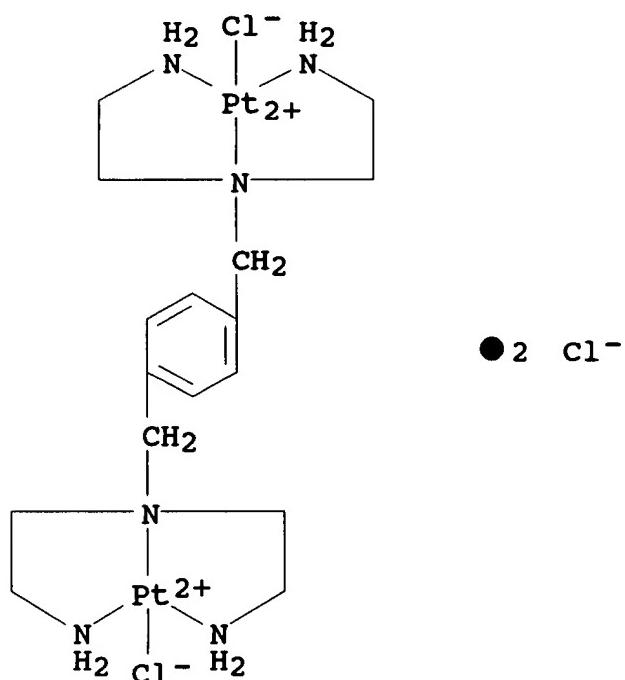
CN Platinum(2+), dichloro[.mu.-[N,N,N',N'-tetrakis(2-aminoethyl)-1,4-benzenedimethanamine-N1,N1',N1'':N4,N4',N4'']]di-, dichloride (9CI)  
(CA INDEX NAME)

MF C16 H32 Cl2 N6 Pt2 . 2 Cl

CI CCS

SR CA

LC STN Files: CA, TOXLIT



## 1 REFERENCES IN FILE CA (1967 TO DATE)

ANSWER 3 REGISTRY COPYRIGHT 1995 ACS

RN 146291-98-7 REGISTRY

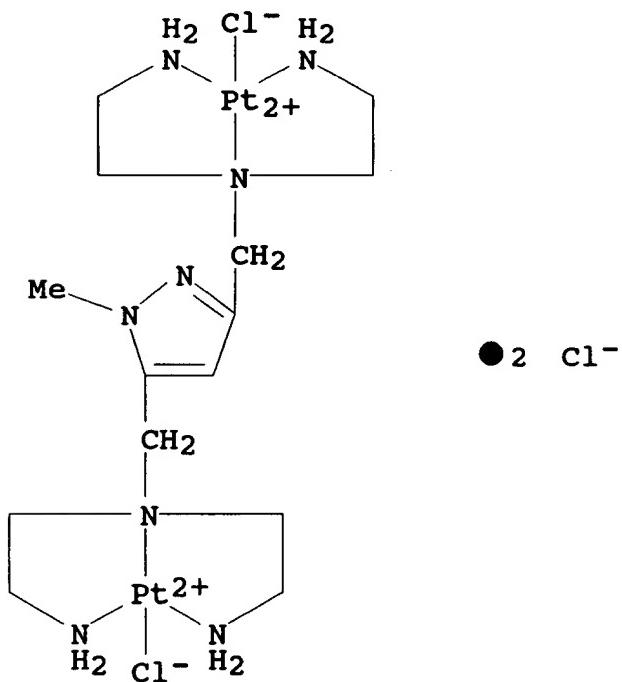
CN Platinum(2+), dichloro[.mu.-[N,N,N',N'-tetrakis(2-aminoethyl)-1-methyl-1H-pyrazole-3,5-dimethanamine-N3,N3',N3'':N5,N5',N5'']]di-, dichloride (9CI) (CA INDEX NAME)

MF C14 H32 Cl2 N8 Pt2 . 2 Cl

CI CCS

SR CA

LC STN Files: CA, TOXLIT



## 1 REFERENCES IN FILE CA (1967 TO DATE)

=> fil ca

FILE 'CA' ENTERED AT 14:10:51 ON 25 MAR 95  
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FILE COVERS 1967 - 18 Mar 1995 (950318/ED) VOL 122 ISS 12

To help control your online searching costs, consider using the HCA File when using the FSEARCH command or when conducting SmartSELECT searches with large numbers of terms.

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=>

=> d all 2

L33 ANSWER 2 OF 2 CA COPYRIGHT 1995 ACS

AN 97:119531 CA

TI Three-coordinate binuclear copper(I) complex: model compound for the copper sites in deoxyhemocyanin and deoxytyrosinase

AU Karlin, Kenneth D.; Gultneh, Yilma; Hutchinson, John P.; Zubietta, Jon

CS Cent. Biol. Macromol., State Univ. New York, Albany, NY, 12222, USA

SO J. Am. Chem. Soc. (1982), 104(19), 5240-2  
CODEN: JACSAT; ISSN: 0002-7863

DT Journal

LA English

CC 78-7 (Inorganic Chemicals and Reactions)  
Section cross-reference(s): 1, 75

OS CJACS

AB The deoxy-binuclear Cu contg. active sites in the dioxygen carrier hemocyanin and the monooxygenase tyrosinase are thought to contain 2 Cu(I) ions in close proximity which are each 2 or 3 coordinate and ligated to nitrogenous ligands. The synthesis and x-ray structural characterization of [Cu<sub>2</sub>L](PF<sub>6</sub>)<sub>2</sub> (I) (L = 1,3-[ (RCH<sub>2</sub>CH<sub>2</sub>)<sub>2</sub>NCH<sub>2</sub>]<sub>2</sub>C<sub>6</sub>H<sub>4</sub>, where = pyridyl) which mimics features of these deoxy sites is described. I contains a binucleating ligand where 2 tridentate groups with pyridyl and amino N-donors are connected by a m-xylyl connecting group. Each crystallog. independent Cu(I) ion is 3-coordinate in a similar distorted trigonal planar geometry with bonding parameters (av.); Cu-N(amino) = 2.16 .ANG.; Cu-N(pyridyl) = 1.92 .ANG.; N(amino)-Cu-N(pyridyl) = 99.8-104.3.degree. N(pyridyl)-Cu-N(pyridyl) = 150.9.degree.. The Cu(I) moieties are extended away from each other; Cu. . . Cu = 8.940(2) .ANG.. I reacts with O in a manner analogous to the monooxygenases; it shows a quasireversible oxidn. wave at E<sub>1/2</sub> = +0.16 V vs. NHE in DMF and reacts with CO and P-contg. ligands.

ST copper pyridylaminoxylyl complex; crystal structure copper pyridylaminoxylyl; xylyl pyridylamino copper complex  
IT Crystal structure  
Molecular structure  
(of copper bis[bis(pyridylethyl)amino]-m-xylyl binuclear complex)

IT 82731-39-3P

(prepn. and crystal structure of)

IT 64443-05-6

(reaction of, with bis[bis(pyridylethyl)amino]-m-xylyl)

=> fil reg ;d 82731-39-3

FILE 'REGISTRY' ENTERED AT 14:11:13 ON 25 MAR 95  
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STRUCTURE FILE UPDATES: 24 MAR 95 HIGHEST RN 161753-30-6  
 DICTIONARY FILE UPDATES: 24 MAR 95 HIGHEST RN 161753-30-6

TSCA INFORMATION NOW CURRENT THROUGH MAY 1994

Please note that search-term pricing does apply when  
 conducting SmartSELECT searches.

ANSWER 1 REGISTRY COPYRIGHT 1995 ACS

RN 82731-39-3 REGISTRY

CN Copper(2+), [.mu.-[N,N,N',N'-tetrakis[2-(2-pyridinyl)ethyl]-1,3-benzenedimethanamine-N1,N1',N1'':N3,N3',N3'']]di-, bis[hexafluorophosphate(1-)] (9CI) (CA INDEX NAME)

OTHER CA INDEX NAMES:

CN 1,3-Benzenedimethanamine, N,N,N',N'-tetrakis[2-(2-pyridinyl)ethyl]-, copper complex

CN Phosphate(1-), hexafluoro-, [.mu.-[N,N,N',N'-tetrakis[2-(2-pyridinyl)ethyl]-1,3-benzenedimethanamine-N1,N1',N1'':N3,N3',N3'']]dicopper(2+) (2:1)

MF C36 H40 Cu2 N6 . 2 F6 P

LC STN Files: CA, CJACS

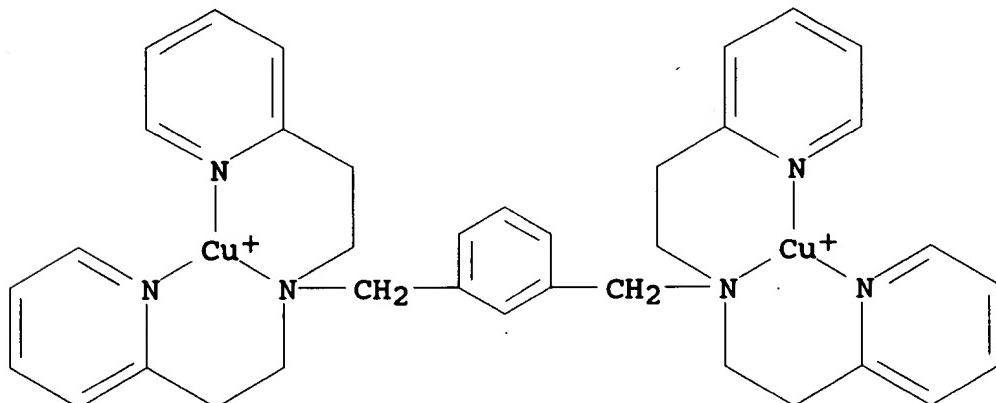
CM 1

CRN 82281-84-3

CMF C36 H40 Cu2 N6

CCI CCS

*These compds are  
in above file*



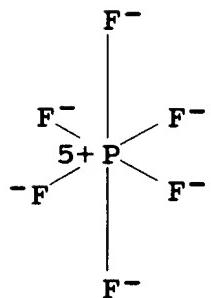
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CM 2

CRN 16919-18-9

CMF F6 P

CCI CCS



2 REFERENCES IN FILE CA (1967 TO DATE)

=> fil reg

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STRUCTURE FILE UPDATES: 24 MAR 95 HIGHEST RN 161753-30-6  
DICTIONARY FILE UPDATES: 24 MAR 95 HIGHEST RN 161753-30-6

TSCA INFORMATION NOW CURRENT THROUGH MAY 1994

Please note that search-term pricing does apply when  
conducting SmartSELECT searches.

=> d que 140

L11 STR

N 1 N 3 N 5

NODE ATTRIBUTES:

NSPEC IS R AT 1

NSPEC IS R AT 3

NSPEC IS R AT 5

DEFAULT MLEVEL IS ATOM

DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED

NUMBER OF NODES IS 3

STEREO ATTRIBUTES: NONE

L13 STR

N—C—Cy—C—N

1 2 3 4 5

NODE ATTRIBUTES:

NSPEC IS R AT 1

NSPEC IS R AT 5

DEFAULT MLEVEL IS ATOM

GGCAT IS UNS AT 3

DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED

NUMBER OF NODES IS 5

STEREO ATTRIBUTES: NONE

L17 STR

Hy—C—Cy—C—Hy

1 2 3 4 5

NODE ATTRIBUTES:

DEFAULT MLEVEL IS ATOM

GGCAT IS HIQ AT 1

GGCAT IS UNS AT 3

GGCAT IS HIQ AT 5

DEFAULT ECLEVEL IS LIMITED  
 ECOUNT IS M4 C M3 N AT 1  
 ECOUNT IS M4 C M3 N AT 5

GRAPH ATTRIBUTES:  
 RING(S) ARE ISOLATED OR EMBEDDED  
 NUMBER OF NODES IS 5

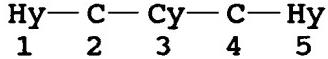
STEREO ATTRIBUTES: NONE  
 L19 STR



NODE ATTRIBUTES:  
 DEFAULT MLEVEL IS ATOM  
 DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:  
 RING(S) ARE ISOLATED OR EMBEDDED  
 NUMBER OF NODES IS 10

STEREO ATTRIBUTES: NONE  
 L22 SCR 1840 AND 1996 AND 140 AND 1607 AND 1236  
 L23 SCR 1840 AND 1996 AND 140 AND 1607 AND 1363  
 L28 308 SEA FILE=REGISTRY SSS FUL L11 AND L13 AND L17 AND L19 AND  
       (L22 OR L23)  
 L36 STR



NODE ATTRIBUTES:  
 DEFAULT MLEVEL IS ATOM  
 GGCAT IS HIQ AT 1  
 GGCAT IS UNS AT 3  
 GGCAT IS HIQ AT 5  
 DEFAULT ECLEVEL IS LIMITED  
 ECOUNT IS M8 C E4 N AT 1  
 ECOUNT IS M8 C E4 N AT 5

GRAPH ATTRIBUTES:  
 RING(S) ARE ISOLATED OR EMBEDDED  
 NUMBER OF NODES IS 5

STEREO ATTRIBUTES: NONE  
 L40 137 SEA FILE=REGISTRY SUB=L28 SSS FUL L36

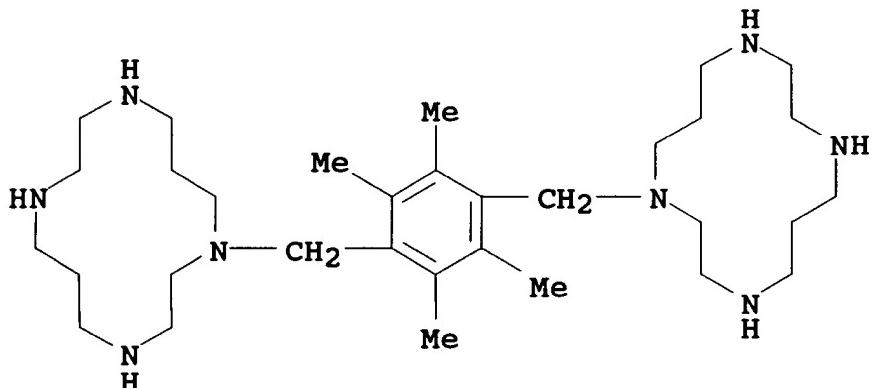
=> d his 141-

(FILE 'REGISTRY' ENTERED AT 14:11:13 ON 25 MAR 95)  
 L41 60 S L38 AND L40  
 L42 STR  
 L43 50 S L42  
 L44 111859 S 591.79.52/RID  
 L45 50 S L43 NOT L41  
 L46 57 S L41 NOT L44

FILE 'REGISTRY' ENTERED AT 14:27:59 ON 25 MAR 95

=> d 1-7 ide can

L46 ANSWER 1 OF 57 REGISTRY COPYRIGHT 1995 ACS  
RN 158200-26-1 REGISTRY  
CN 1,4,8,11-Tetraazacyclotetradecane, 1,1'-(2,3,5,6-tetramethyl-1,4-phenylene)bis(methylene)]bis- (9CI) (CA INDEX NAME)  
FS 3D CONCORD  
MF C32 H62 N8  
SR CA  
LC STN Files: CA

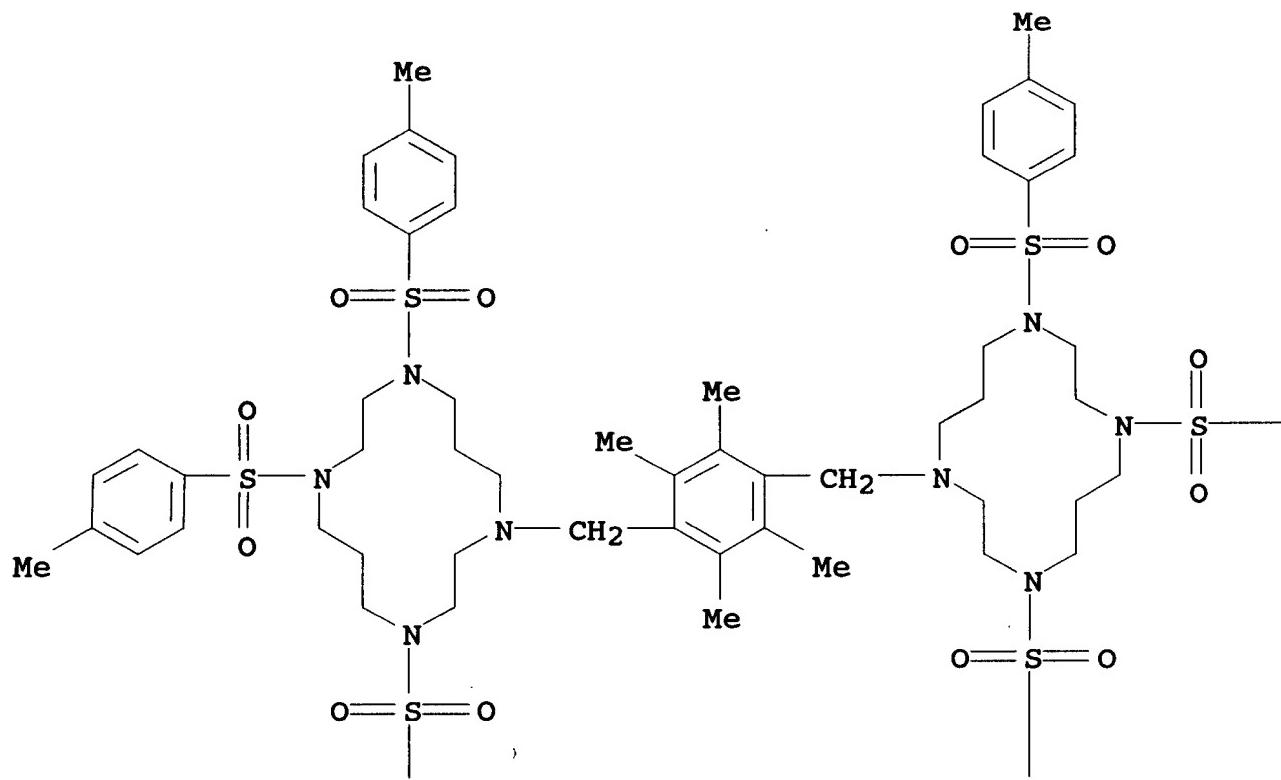


1 REFERENCES IN FILE CA (1967 TO DATE)

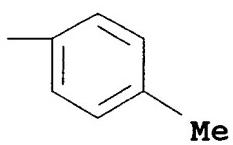
REFERENCE 1: 121:225706

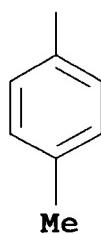
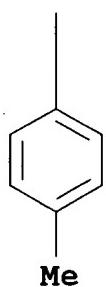
L46 ANSWER 2 OF 57 REGISTRY COPYRIGHT 1995 ACS  
RN 158200-25-0 REGISTRY  
CN 1,4,8,11-Tetraazacyclotetradecane, 1,1'-(2,3,5,6-tetramethyl-1,4-phenylene)bis(methylene)]bis[4,8,11-tris[(4-methylphenyl)sulfonyl]- (9CI) (CA INDEX NAME)  
FS 3D CONCORD  
MF C74 H98 N8 O12 S6  
SR CA  
LC STN Files: CA

PAGE 1-A



PAGE 1-B



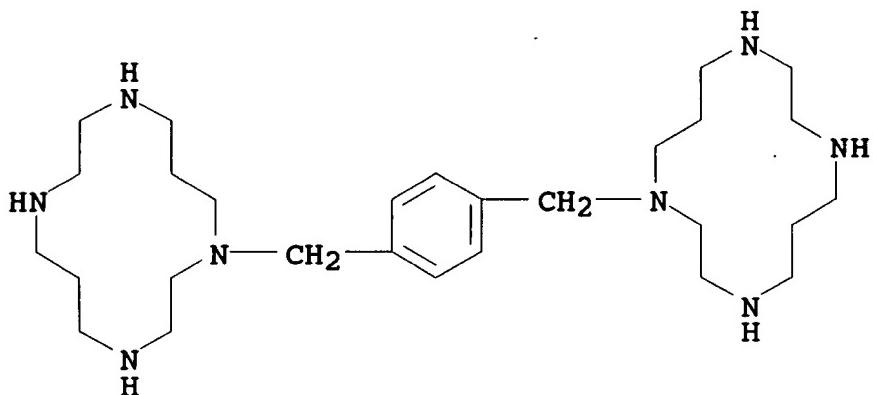


PAGE 2-A

## 1 REFERENCES IN FILE CA (1967 TO DATE)

REFERENCE 1: 121:225706

L46 ANSWER 3 OF 57 REGISTRY COPYRIGHT 1995 ACS  
 RN 155148-32-6 REGISTRY  
 CN 1,4,8,11-Tetraazacyclotetradecane, 1,1'-[1,4-phenylenebis(methylene)]bis-, octahydrobromide (9CI) (CA INDEX NAME)  
 MF C28 H54 N8 . 8 Br H  
 SR CA  
 LC STN Files: CA, TOXLIT  
 CRN (110078-46-1)



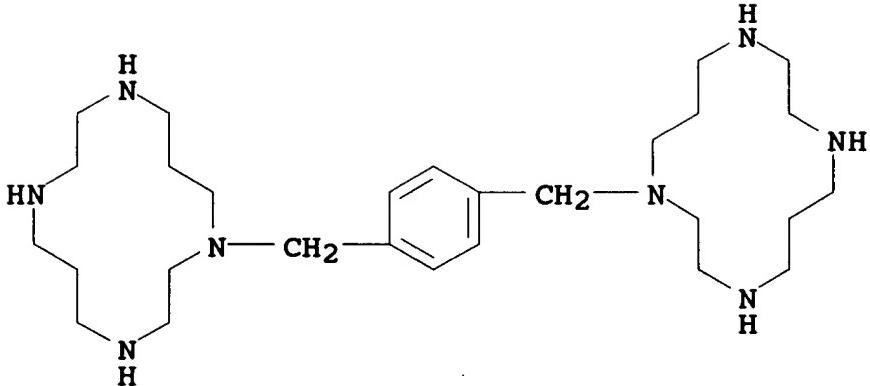
● 8 HBr

## 1 REFERENCES IN FILE CA (1967 TO DATE)

REFERENCE 1: 120:289504

L46 ANSWER 4 OF 57 REGISTRY COPYRIGHT 1995 ACS  
 RN 155148-31-5 REGISTRY  
 CN 1,4,8,11-Tetraazacyclotetradecane, 1,1'-[1,4-phenylenebis(methylene)]bis-, octahydrochloride (9CI) (CA INDEX NAME)  
 MF C28 H54 N8 . 8 Cl H

SR CA  
 LC STN Files: CA, TOXLIT  
 CRN (110078-46-1)



● 8 HCl

1 REFERENCES IN FILE CA (1967 TO DATE)

REFERENCE 1: 120:289504

L46 ANSWER 5 OF 57 REGISTRY COPYRIGHT 1995 ACS  
 RN 151987-13-2 REGISTRY  
 CN Cobalt(2+), [.mu.-[1,1'-[1,8-anthracenediylbis(methylene)]bis[1,4,7,10-tetraazacyclododecane]-N1,N4,N7,N10:N1',N4',N7',N10']]bis[carbonato(2-)O,O']di-, dichloride, stereoisomer (9CI) (CA INDEX NAME)  
 OTHER CA INDEX NAMES:  
 CN 1,4,7,10-Tetraazacyclododecane, cobalt(2+) deriv. (9CI)  
 MF C34 H50 Co2 N8 O6 . 2 Cl  
 CI CCS  
 SR CA  
 LC STN Files: CA  
 DES \*

\*\*\* STRUCTURE DIAGRAM IS NOT AVAILABLE \*\*\*

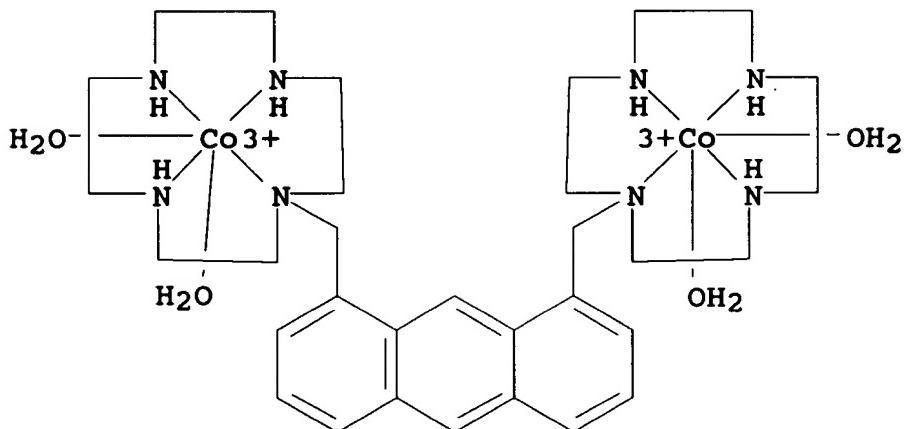
1 REFERENCES IN FILE CA (1967 TO DATE)

REFERENCE 1: 120:44414

L46 ANSWER 6 OF 57 REGISTRY COPYRIGHT 1995 ACS  
 RN 151956-64-8 REGISTRY  
 CN Cobalt(6+), [.mu.-[1,1'-[1,8-anthracenediylbis(methylene)]bis[1,4,7,10-tetraazacyclododecane]-N1,N4,N7,N10:N1',N4',N7',N10']]tetraaquadi-, stereoisomer, hexanitrate (9CI) (CA INDEX NAME)  
 OTHER CA INDEX NAMES:  
 CN 1,4,7,10-Tetraazacyclododecane, cobalt(6+) deriv. (9CI)  
 MF C32 H58 Co2 N8 O4 . 6 N O3  
 SR CA  
 LC STN Files: CA

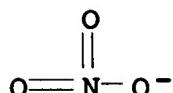
CM 1

CRN 151956-63-7  
 CMF C32 H58 Co2 N8 O4  
 CCI CCS  
 CDES \*



CM 2

CRN 14797-55-8  
 CMF N O3



## 1 REFERENCES IN FILE CA (1967 TO DATE)

REFERENCE 1: 120:44414

L46 ANSWER 7 OF 57 REGISTRY COPYRIGHT 1995 ACS

RN 151956-63-7 REGISTRY

CN Cobalt(6+), [.mu.-[1,1'-[1,8-anthracenediylbis(methylene)]bis[1,4,7,10-tetraazacyclododecane]-N1,N4,N7,N10:N1',N4',N7',N10']]tetraaquadi-, stereoisomer (9CI) (CA INDEX NAME)

## OTHER CA INDEX NAMES:

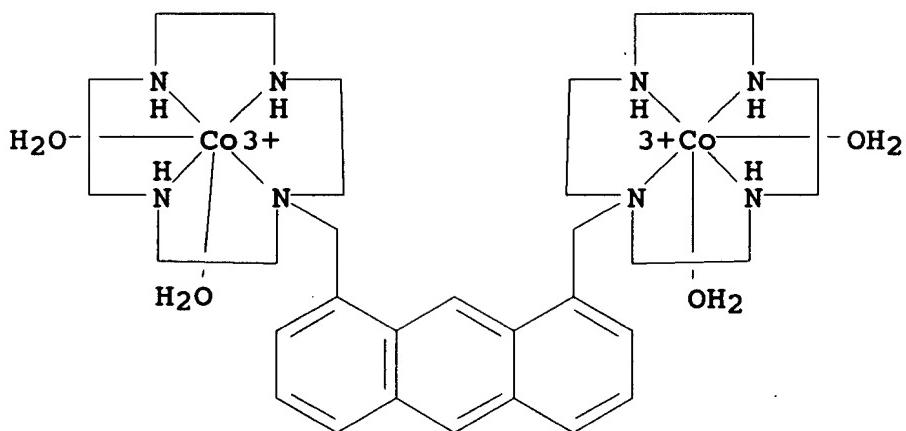
CN 1,4,7,10-Tetraazacyclododecane, cobalt(6+) deriv. (9CI)

MF C32 H58 Co2 N8 O4

CI CCS, COM

SR CA

DES \*



=> d 8-30 ide can

L46 ANSWER 8 OF 57 REGISTRY COPYRIGHT 1995 ACS

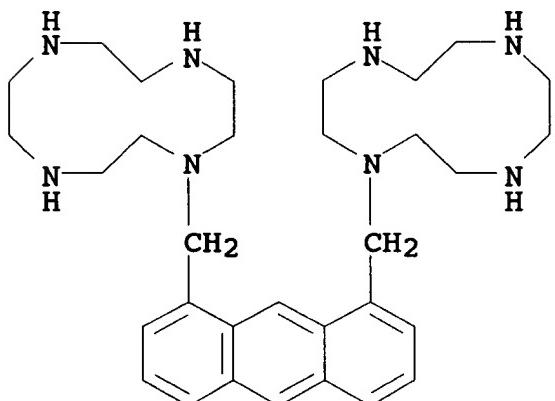
RN 151697-44-8 REGISTRY

CN 1,4,7,10-Tetraazacyclododecane, 1,1'-[1,8-anthracenediyylbis(methylene)]bis-, octahydrochloride (9CI) (CA INDEX NAME)

MF C32 H50 N8 . 8 Cl H

SR CA

LC STN Files: CA



● 8 HCl

#### 1 REFERENCES IN FILE CA (1967 TO DATE)

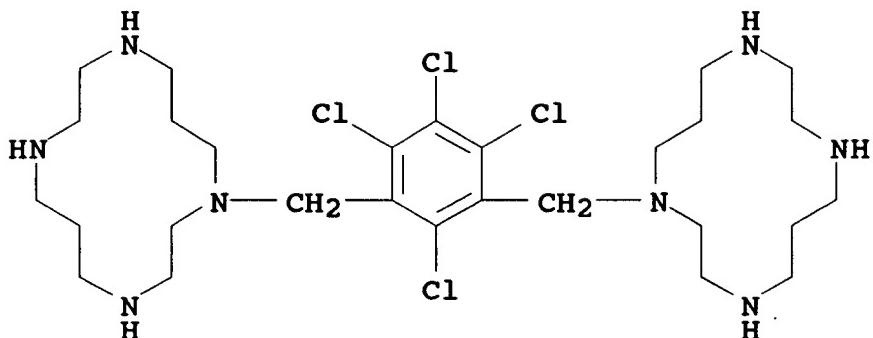
REFERENCE 1: 120:44414

L46 ANSWER 9 OF 57 REGISTRY COPYRIGHT 1995 ACS

RN 151191-34-3 REGISTRY

CN 1,4,8,11-Tetraazacyclotetradecane, 1,1'-(2,4,5,6-tetrachloro-1,3-phenylene)bis(methylene)]bis- (9CI) (CA INDEX NAME)

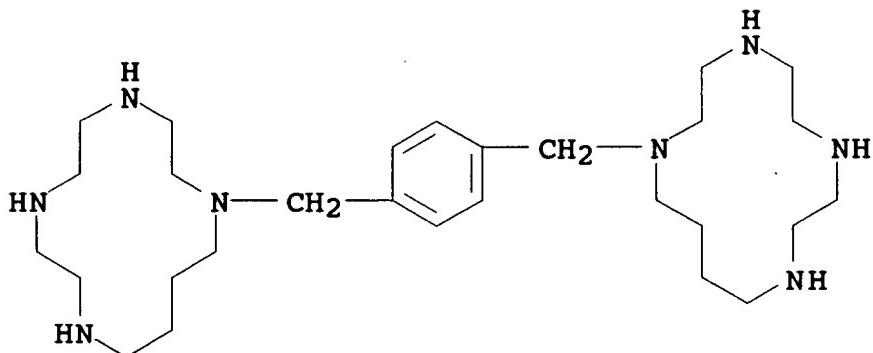
FS 3D CONCORD  
 MF C28 H50 Cl4 N8  
 CI COM  
 SR CA  
 LC STN Files: CA



1 REFERENCES IN FILE CA (1967 TO DATE)

REFERENCE 1: P 120:30786

L46 ANSWER 10 OF 57 REGISTRY COPYRIGHT 1995 ACS  
 RN 151191-33-2 REGISTRY  
 CN 1,4,7,10-Tetraazacyclotetradecane, 1,1'-[1,4-  
 phenylenebis(methylene)]bis- (9CI) (CA INDEX NAME)  
 FS 3D CONCORD  
 MF C28 H54 N8  
 SR CA  
 LC STN Files: CA

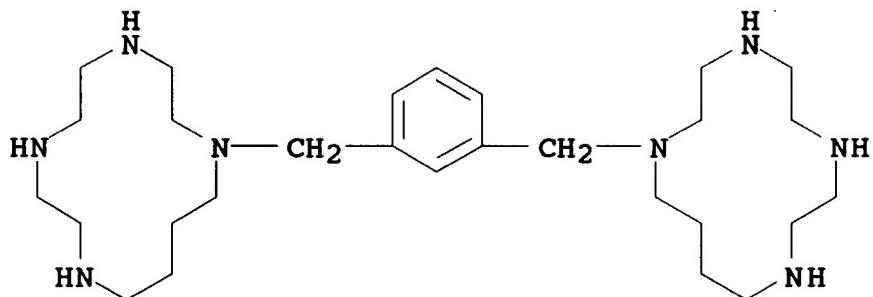


1 REFERENCES IN FILE CA (1967 TO DATE)

REFERENCE 1: P 120:30786

L46 ANSWER 11 OF 57 REGISTRY COPYRIGHT 1995 ACS  
 RN 151191-32-1 REGISTRY  
 CN 1,4,7,10-Tetraazacyclotetradecane, 1,1'-[1,3-  
 phenylenebis(methylene)]bis- (9CI) (CA INDEX NAME)  
 FS 3D CONCORD  
 MF C28 H54 N8

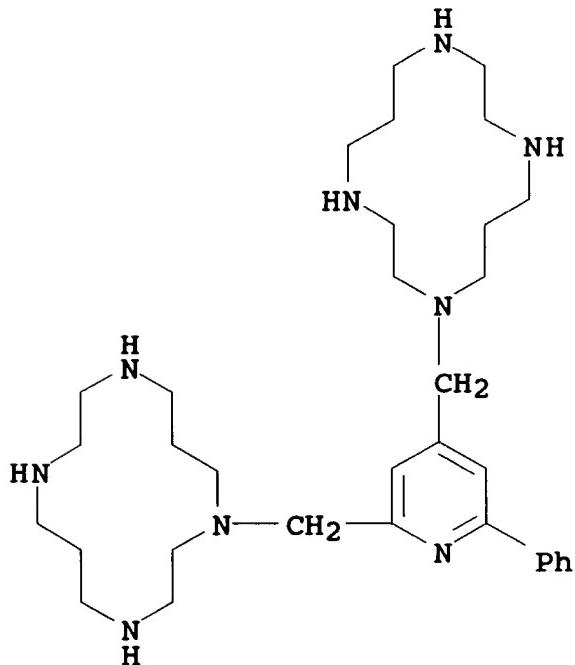
SR CA  
 LC STN Files: CA



1 REFERENCES IN FILE CA (1967 TO DATE)

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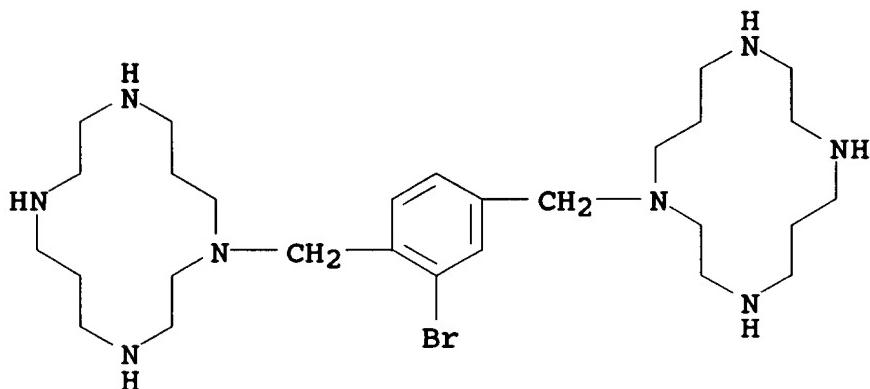
L46 ANSWER 12 OF 57 REGISTRY COPYRIGHT 1995 ACS  
 RN 151191-31-0 REGISTRY  
 CN 1,4,8,11-Tetraazacyclotetradecane, 1,1'-[ (6-phenyl-2,4-pyridinediyl)bis(methylene) ]bis- (9CI) (CA INDEX NAME)  
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 MF C33 H57 N9  
 SR CA  
 LC STN Files: CA



1 REFERENCES IN FILE CA (1967 TO DATE)

REFERENCE 1: P 120:30786

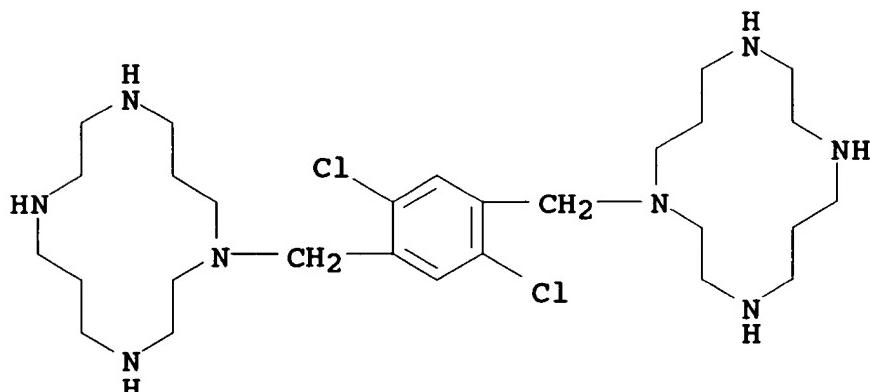
L46 ANSWER 13 OF 57 REGISTRY COPYRIGHT 1995 ACS  
 RN 151191-30-9 REGISTRY  
 CN 1,4,8,11-Tetraazacyclotetradecane, 1,1'-[ (2-bromo-1,4-phenylene)bis(methylene)]bis- (9CI) (CA INDEX NAME)  
 FS 3D CONCORD  
 MF C28 H53 Br N8  
 SR CA  
 LC STN Files: CA



1 REFERENCES IN FILE CA (1967 TO DATE)

REFERENCE 1: P 120:30786

L46 ANSWER 14 OF 57 REGISTRY COPYRIGHT 1995 ACS  
 RN 151191-29-6 REGISTRY  
 CN 1,4,8,11-Tetraazacyclotetradecane, 1,1'-[ (2,5-dichloro-1,4-phenylene)bis(methylene)]bis- (9CI) (CA INDEX NAME)  
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 MF C28 H52 Cl2 N8  
 SR CA  
 LC STN Files: CA

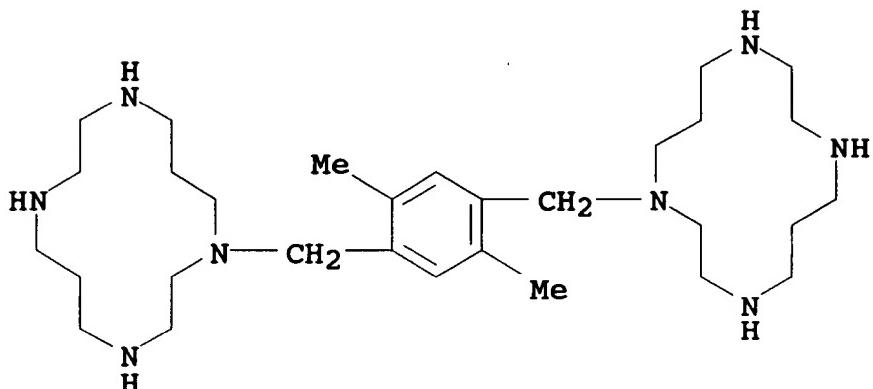


1 REFERENCES IN FILE CA (1967 TO DATE)

REFERENCE 1: P 120:30786

L46 ANSWER 15 OF 57 REGISTRY COPYRIGHT 1995 ACS

RN 151191-28-5 REGISTRY  
CN 1,4,8,11-Tetraazacyclotetradecane, 1,1'-(2,5-dimethyl-1,4-phenylene)bis(methylene)bis- (9CI) (CA INDEX NAME)  
FS 3D CONCORD  
MF C30 H58 N8  
SR CA  
LC STN Files: CA

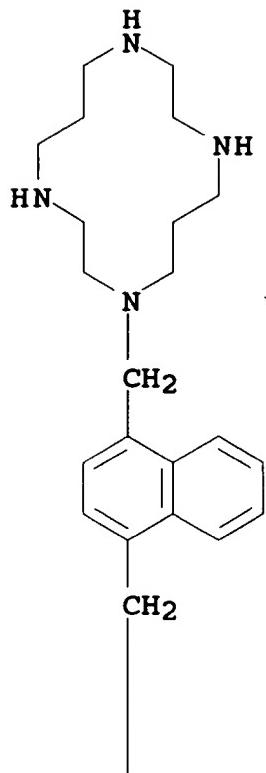


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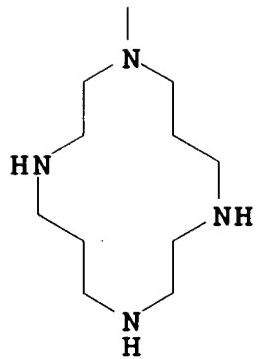
REFERENCE 1: P 120:30786

L46 ANSWER 16 OF 57 REGISTRY COPYRIGHT 1995 ACS  
RN 151191-27-4 REGISTRY  
CN 1,4,8,11-Tetraazacyclotetradecane, 1,1'-(1,4-naphthalenediyl)bis(methylene)bis- (9CI) (CA INDEX NAME)  
FS 3D CONCORD  
MF C32 H56 N8  
CI COM  
SR CA  
LC STN Files: CA

PAGE 1-A



PAGE 2-A

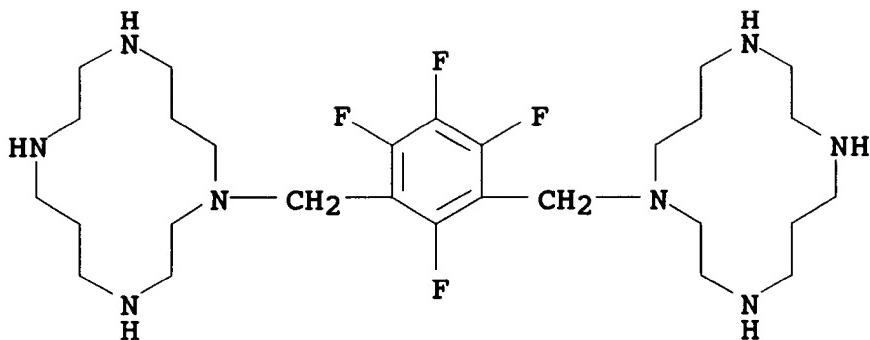


## 1 REFERENCES IN FILE CA (1967 TO DATE)

REFERENCE 1: P 120:30786

L46 ANSWER 17 OF 57 REGISTRY COPYRIGHT 1995 ACS  
RN 151191-26-3 REGISTRY  
CN 1,4,8,11-Tetraazacyclotetradecane, 1,1'-[ (2,4,5,6-tetrafluoro-1,3-phenylene)bis(methylene)]bis- (9CI) (CA INDEX NAME)  
FS 3D CONCORD  
MF C28 H50 F4 N8  
SR CA

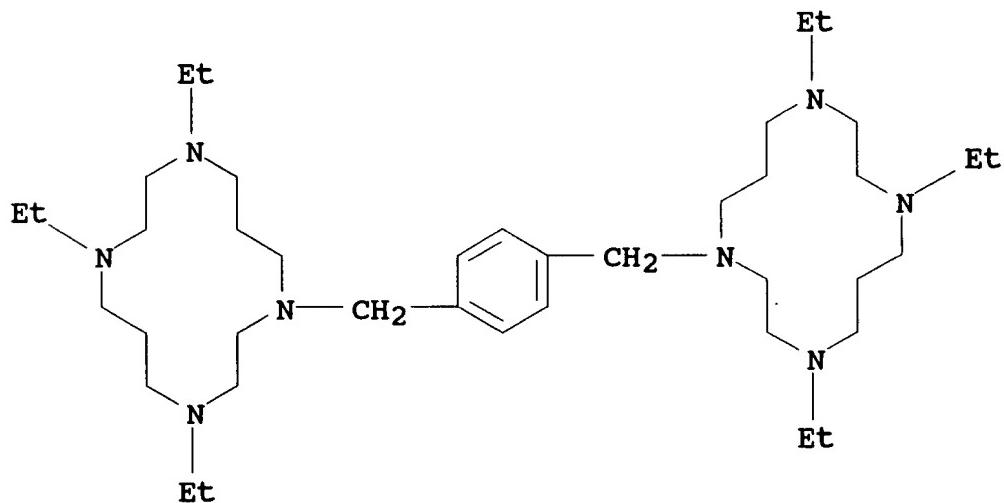
LC STN Files: CA



## 1 REFERENCES IN FILE CA (1967 TO DATE)

REFERENCE 1: P 120:30786

L46 ANSWER 18 OF 57 REGISTRY COPYRIGHT 1995 ACS  
 RN 151191-21-8 REGISTRY  
 CN 1,4,8,11-Tetraazacyclotetradecane, 1,1'-[1,4-phenylenebis(methylene)]bis[4,8,11-triethyl- (9CI) (CA INDEX NAME)  
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 MF C40 H78 N8  
 CI COM  
 SR CA  
 LC STN Files: CA

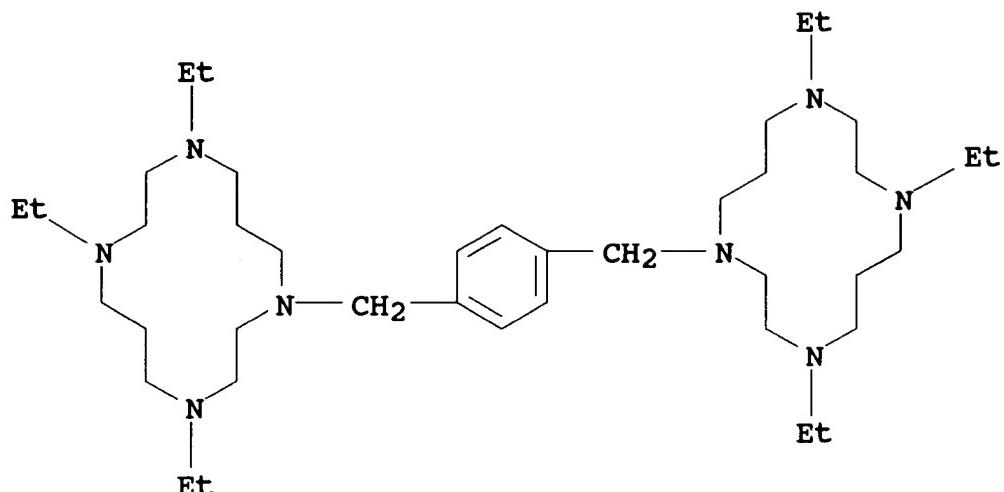


## 1 REFERENCES IN FILE CA (1967 TO DATE)

REFERENCE 1: P 120:30786

L46 ANSWER 19 OF 57 REGISTRY COPYRIGHT 1995 ACS  
 RN 151191-20-7 REGISTRY  
 CN 1,4,8,11-Tetraazacyclotetradecane, 1,1'-[1,4-phenylenebis(methylene)]bis[4,8,11-triethyl-, octahydrobromide (9CI)

(CA INDEX NAME)  
MF C40 H78 N8 . 8 Br H  
SR CA  
LC STN Files: CA  
CRN (151191-21-8)

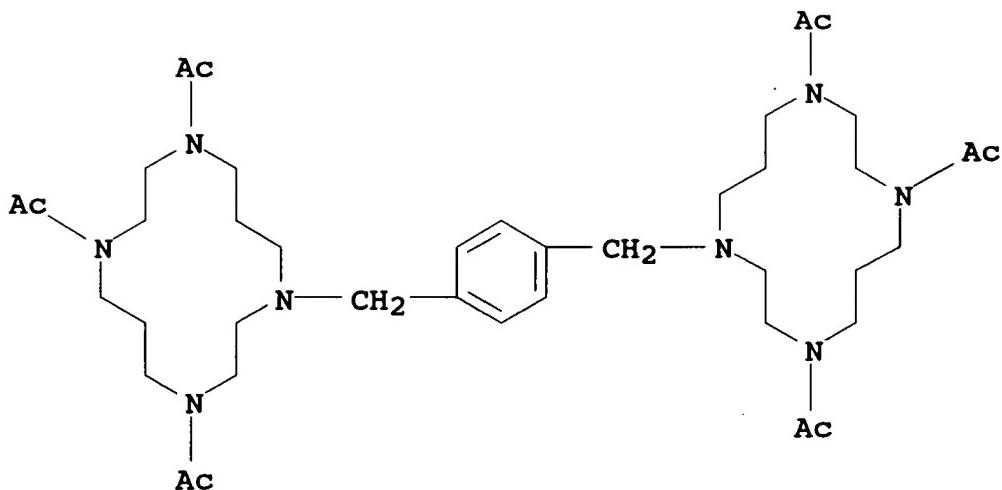


● 8 HBr

1 REFERENCES IN FILE CA (1967 TO DATE)

REFERENCE 1: P 120:30786

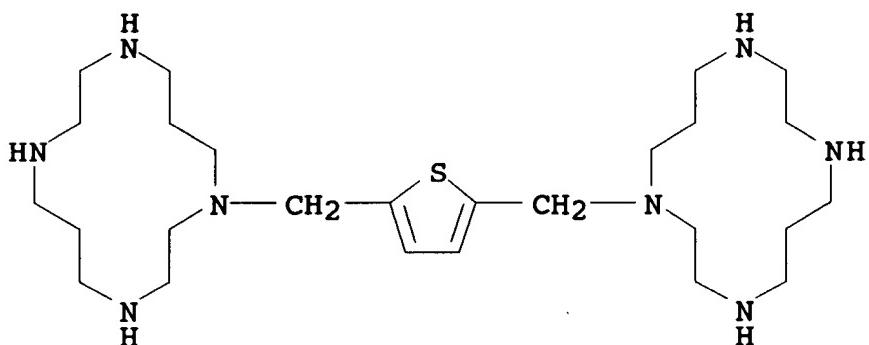
L46 ANSWER 20 OF 57 REGISTRY COPYRIGHT 1995 ACS  
RN 151191-19-4 REGISTRY  
CN 1,4,8,11-Tetraazacyclotetradecane, 1,1'-[1,4-phenylenebis(methylene)]bis[4,8,11-triacetyl- (9CI) (CA INDEX NAME)  
FS 3D CONCORD  
MF C40 H66 N8 O6  
SR CA  
LC STN Files: CA



## 1 REFERENCES IN FILE CA (1967 TO DATE)

REFERENCE 1: P 120:30786

L46 ANSWER 21 OF 57 REGISTRY COPYRIGHT 1995 ACS  
 RN 151191-18-3 REGISTRY  
 CN 1,4,8,11-Tetraazacyclotetradecane, 1,1'-(2,5-thiophenediyl)bis(methylene)bis- (9CI) (CA INDEX NAME)  
 FS 3D CONCORD  
 MF C26 H52 N8 S  
 CI COM  
 SR CA  
 LC STN Files: CA

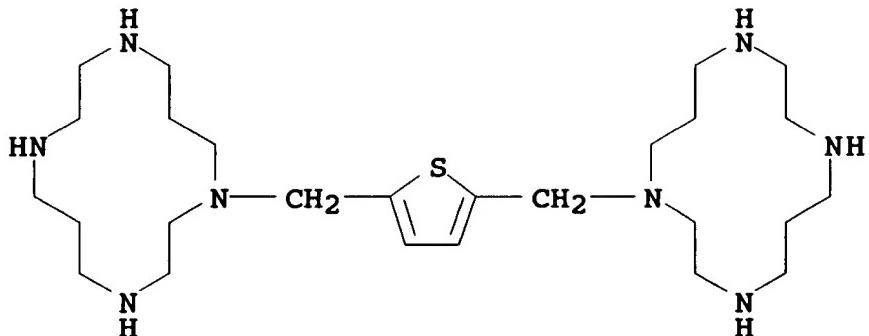


## 1 REFERENCES IN FILE CA (1967 TO DATE)

REFERENCE 1: P 120:30786

L46 ANSWER 22 OF 57 REGISTRY COPYRIGHT 1995 ACS  
 RN 151191-17-2 REGISTRY  
 CN 1,4,8,11-Tetraazacyclotetradecane, 1,1'-(2,5-thiophenediyl)bis(methylene)bis-, octahydrobromide (9CI) (CA INDEX NAME)  
 MF C26 H52 N8 S . 8 Br H

SR CA  
LC STN Files: CA  
CRN (151191-18-3)



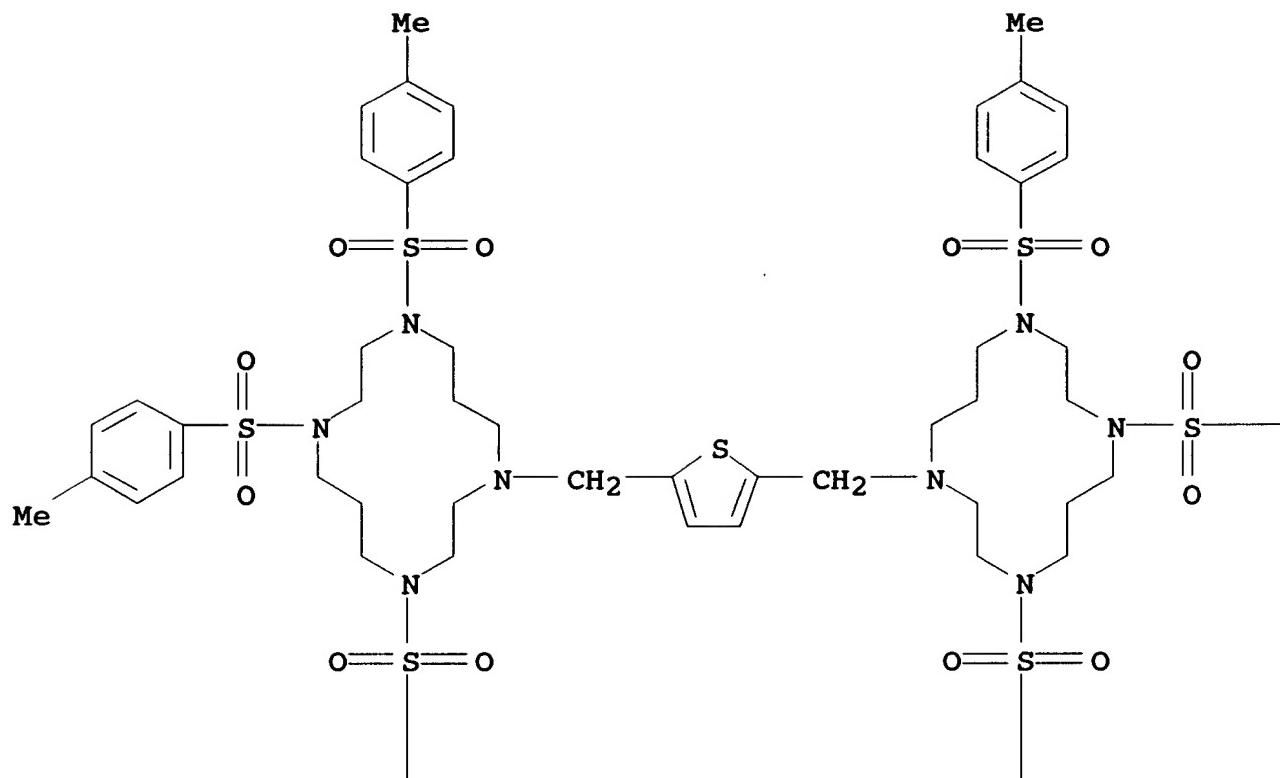
● 8 HBr

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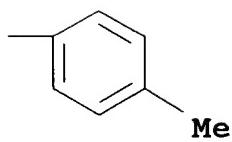
REFERENCE 1: P 120:30786

L46 ANSWER 23 OF 57 REGISTRY COPYRIGHT 1995 ACS  
RN 151191-16-1 REGISTRY  
CN 1,4,8,11-Tetraazacyclotetradecane, 1,1'-[2,5-thiophenediyli]bis(methylene)bis[4,8,11-tris[(4-methylphenyl)sulfonyl]- (9CI) (CA INDEX NAME)  
FS 3D CONCORD  
MF C68 H88 N8 O12 S7  
SR CA  
LC STN Files: CA

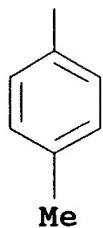
PAGE 1-A



PAGE 1-B



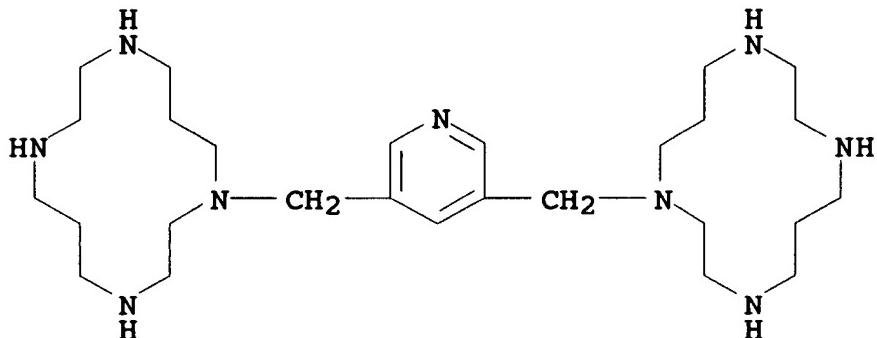
PAGE 2-A



## 1 REFERENCES IN FILE CA (1967 TO DATE)

REFERENCE 1: P 120:30786

L46 ANSWER 24 OF 57 REGISTRY COPYRIGHT 1995 ACS  
 RN 151191-09-2 REGISTRY  
 CN 1,4,8,11-Tetraazacyclotetradecane, 1,1'-[3,5-pyridinediylbis(methylene)]bis- (9CI) (CA INDEX NAME)  
 FS 3D CONCORD  
 MF C27 H53 N9  
 CI COM  
 SR CA  
 LC STN Files: CA, TOXLIT

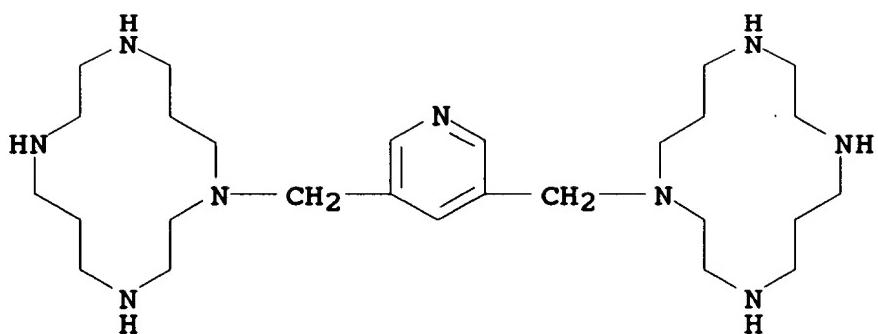


## 2 REFERENCES IN FILE CA (1967 TO DATE)

REFERENCE 1: 120:289504

REFERENCE 2: P 120:30786

L46 ANSWER 25 OF 57 REGISTRY COPYRIGHT 1995 ACS  
 RN 151191-08-1 REGISTRY  
 CN 1,4,8,11-Tetraazacyclotetradecane, 1,1'-[3,5-pyridinediylbis(methylene)]bis-, nonahydrobromide (9CI) (CA INDEX NAME)  
 MF C27 H53 N9 . 9 Br H  
 SR CA  
 LC STN Files: CA  
 CRN (151191-09-2)



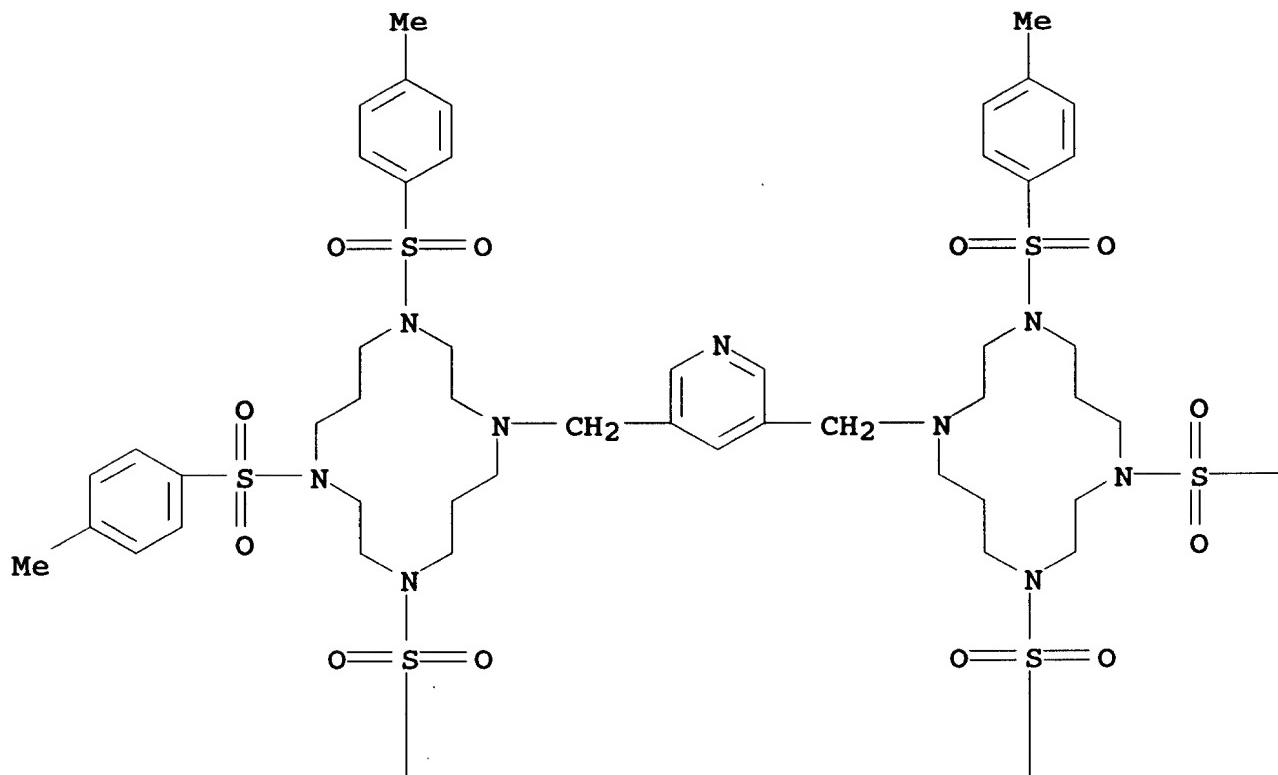
● 9 HBr

1 REFERENCES IN FILE CA (1967 TO DATE)

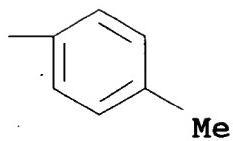
REFERENCE 1: P 120:30786

L46 ANSWER 26 OF 57 REGISTRY COPYRIGHT 1995 ACS  
RN 151191-07-0 REGISTRY  
CN 1,4,8,11-Tetraazacyclotetradecane, 1,1'-(3,5-pyridinediyl)bis(methylene)bis[4,8,11-tris[(4-methylphenyl)sulfonyl]- (9CI) (CA INDEX NAME)  
FS 3D CONCORD  
MF C69 H89 N9 O12 S6  
SR CA  
LC STN Files: CA

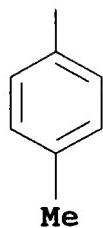
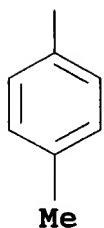
PAGE 1-A



PAGE 1-B



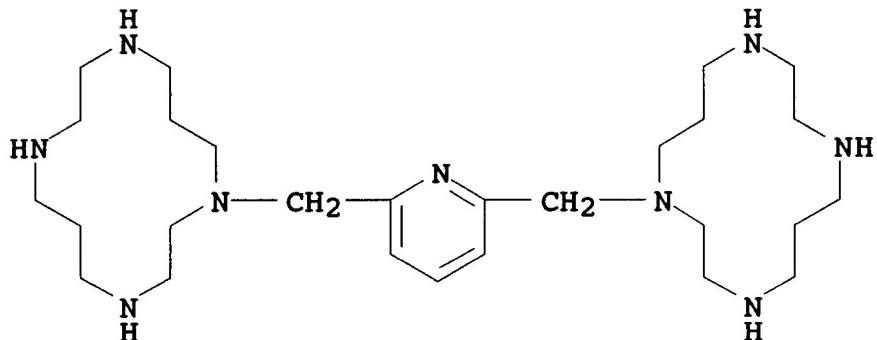
PAGE 2-A



## 1 REFERENCES IN FILE CA (1967 TO DATE)

REFERENCE 1: P 120:30786

L46 ANSWER 27 OF 57 REGISTRY COPYRIGHT 1995 ACS  
 RN 151191-06-9 REGISTRY  
 CN 1,4,8,11-Tetraazacyclotetradecane, 1,1'-[2,6-pyridinediylbis(methylene)]bis- (9CI) (CA INDEX NAME)  
 FS 3D CONCORD  
 MF C27 H53 N9  
 CI COM  
 SR CA  
 LC STN Files: CA, TOXLIT

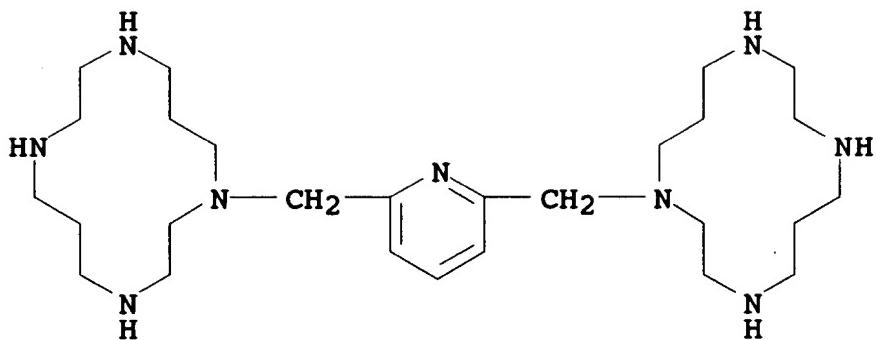


## 2 REFERENCES IN FILE CA (1967 TO DATE)

REFERENCE 1: 120:289504

REFERENCE 2: P 120:30786

L46 ANSWER 28 OF 57 REGISTRY COPYRIGHT 1995 ACS  
 RN 151191-05-8 REGISTRY  
 CN 1,4,8,11-Tetraazacyclotetradecane, 1,1'-[2,6-pyridinediylbis(methylene)]bis-, octahydrobromide (9CI) (CA INDEX NAME)  
 MF C27 H53 N9 . 8 Br H  
 SR CA  
 LC STN Files: CA  
 CRN (151191-06-9)



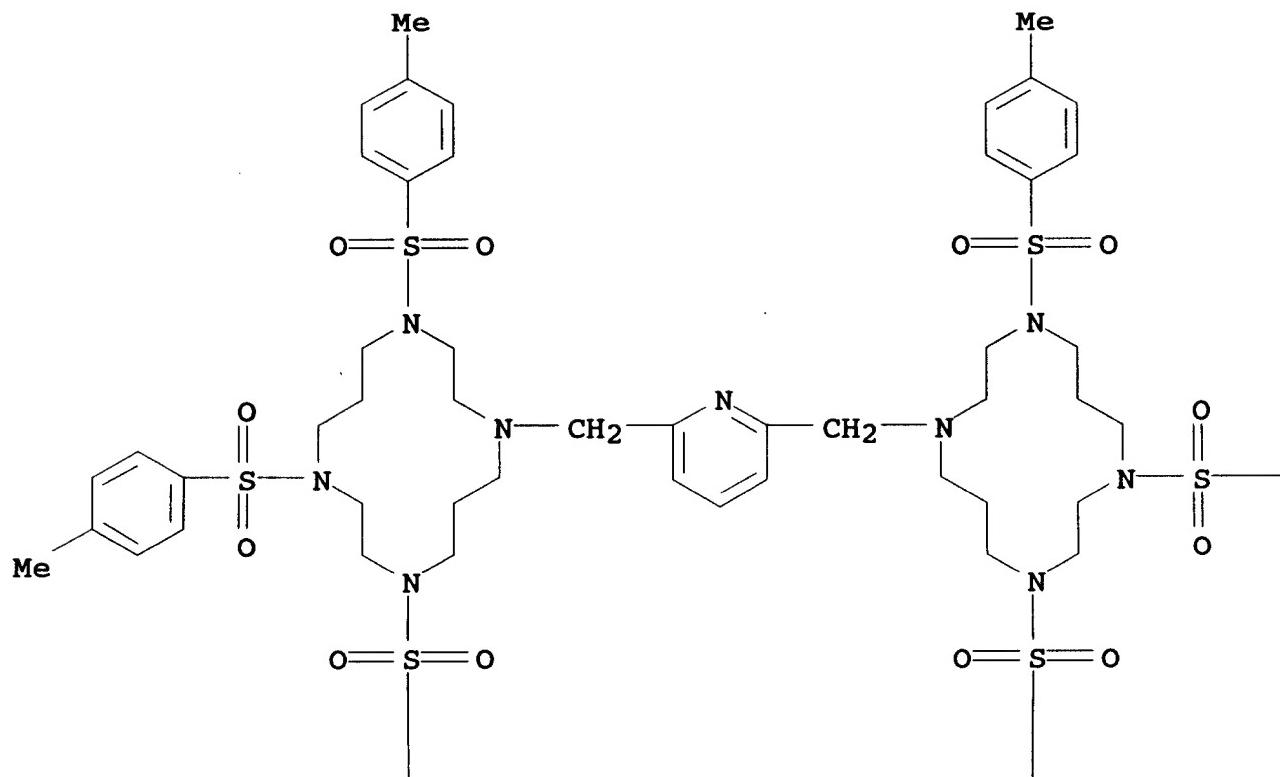
## ● 8 HBr

## 1 REFERENCES IN FILE CA (1967 TO DATE)

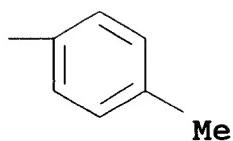
REFERENCE 1: P 120:30786

L46 ANSWER 29 OF 57 REGISTRY COPYRIGHT 1995 ACS  
RN 151191-04-7 REGISTRY  
CN 1,4,8,11-Tetraazacyclotetradecane, 1,1'-(2,6-pyridinediyl)bis(methylene)bis[4,8,11-tris[(4-methylphenyl)sulfonyl]- (9CI) (CA INDEX NAME)  
FS 3D CONCORD  
MF C69 H89 N9 O12 S6  
SR CA  
LC STN Files: CA

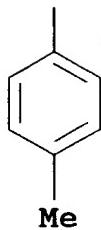
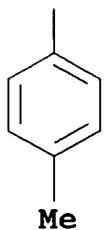
PAGE 1-A



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## 1 REFERENCES IN FILE CA (1967 TO DATE)

REFERENCE 1: P 120:30786

L46 ANSWER 30 OF 57 REGISTRY COPYRIGHT 1995 ACS

RN 151191-03-6 REGISTRY

CN 1,4,7,11-Tetraazacyclotetradecane, 11-[[4-(1,4,8,11-tetraazacyclotetradec-1-ylmethyl)phenyl]methyl]- (9CI) (CA INDEX NAME)

OTHER CA INDEX NAMES:

CN 1,4,8,11-Tetraazacyclotetradecane, 1,4,7,11-tetraazacyclotetradecane deriv. (9CI)

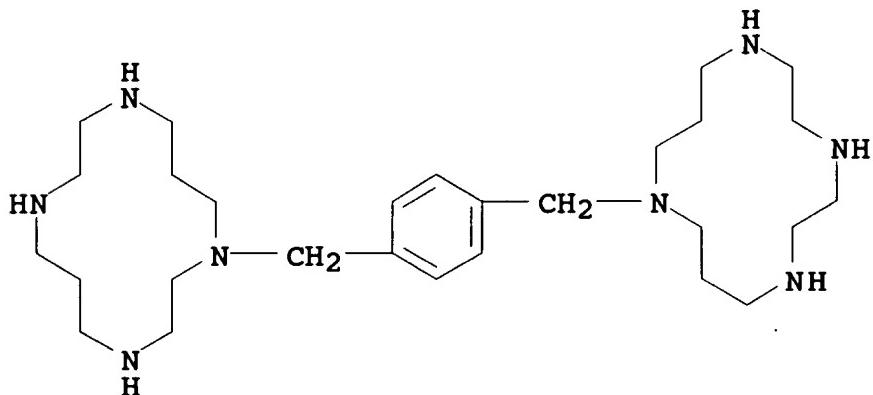
FS 3D CONCORD

MF C28 H54 N8

CI COM

SR CA

LC STN Files: CA



## 1 REFERENCES IN FILE CA (1967 TO DATE)

REFERENCE 1: P 120:30786

=&gt; d ide can 50-57

L46 ANSWER 50 OF 57 REGISTRY COPYRIGHT 1995 ACS

RN 142079-95-6 REGISTRY

CN Iron(2+), tris[1-((2,2'-bipyridin)-5-ylmethyl)-1,4,8,11-tetraazacyclotetradecane]-, (OC-6-21)- (9CI) (CA INDEX NAME)

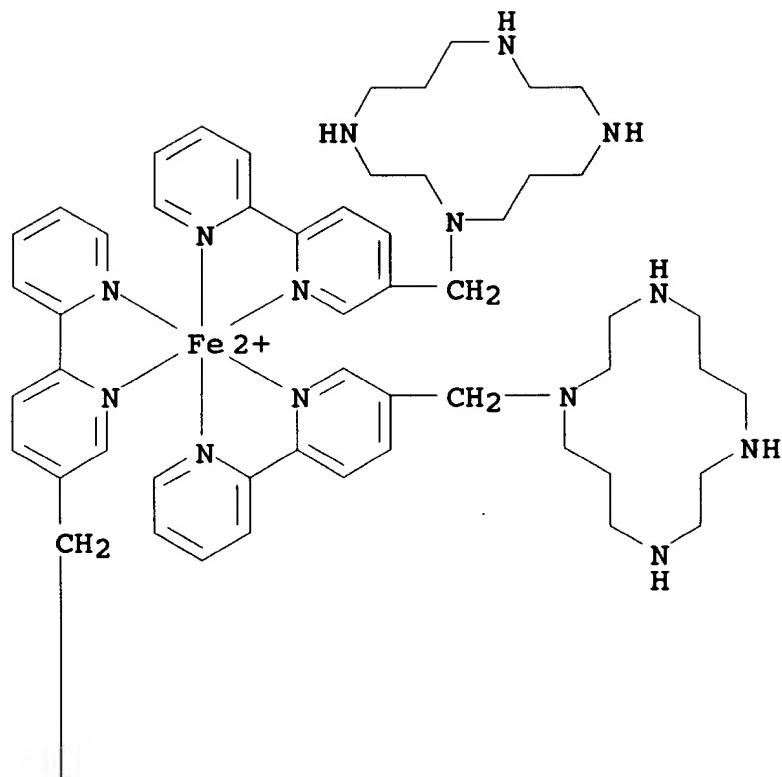
OTHER CA INDEX NAMES:

CN 1,4,8,11-Tetraazacyclotetradecane, iron(2+) deriv. (9CI)

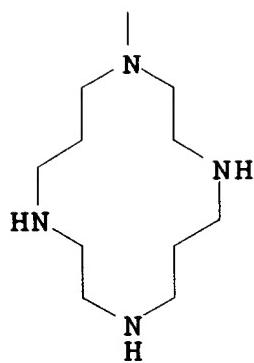
MF C63 H96 Fe N18

CI CCS  
SR CA  
LC STN Files: CA  
DES 7:OC-6-21

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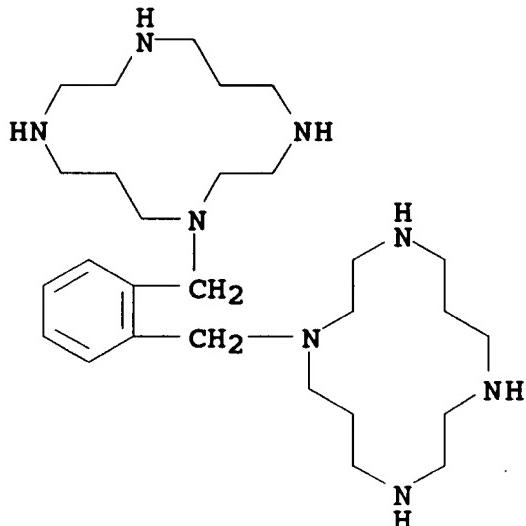


1 REFERENCES IN FILE CA (1967 TO DATE)

REFERENCE 1: 117:82274

L46 ANSWER 51 OF 57 REGISTRY COPYRIGHT 1995 ACS  
RN 133563-60-7 REGISTRY

CN 1,4,8,11-Tetraazacyclotetradecane, 1,1'-[1,2-phenylenebis(methylene)]bis- (9CI) (CA INDEX NAME)  
FS 3D CONCORD  
MF C28 H54 N8  
SR CA  
LC STN Files: CA, USPATFULL

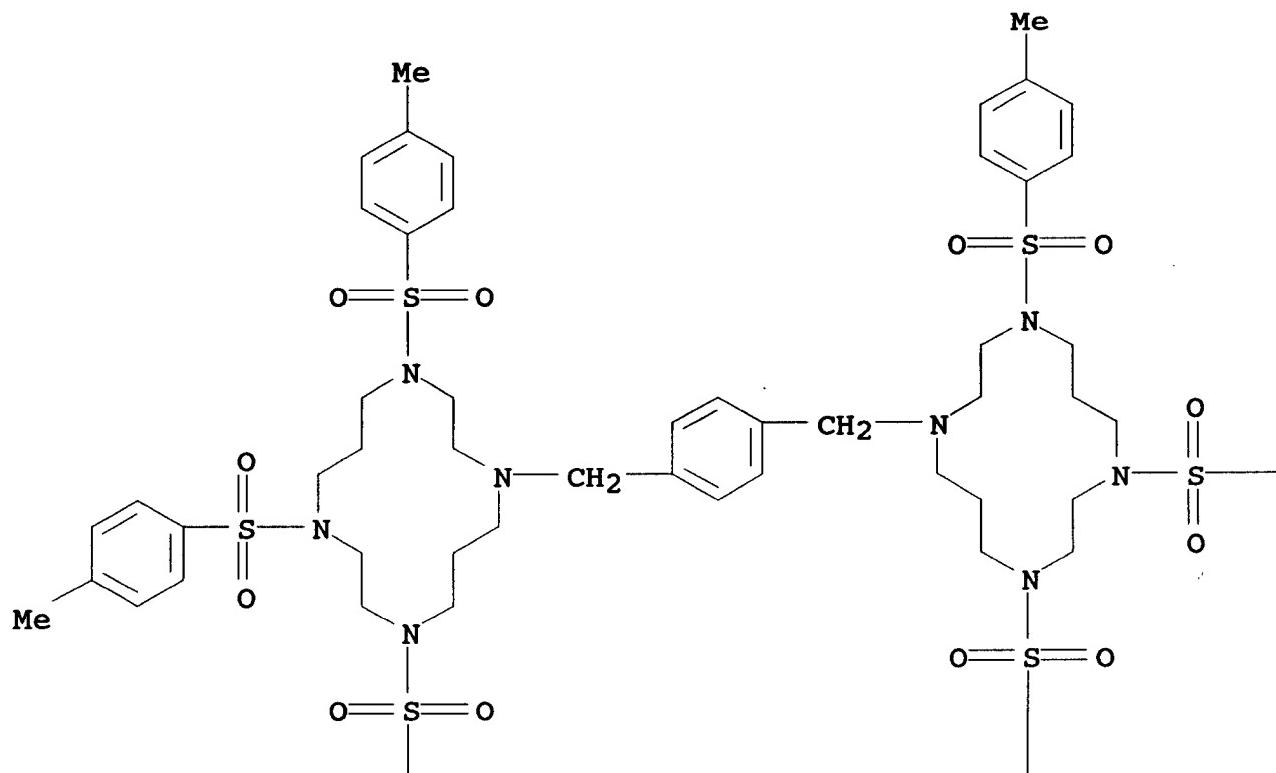


## 1 REFERENCES IN FILE CA (1967 TO DATE)

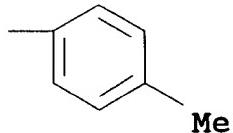
REFERENCE 1: P 114:207294

L46 ANSWER 52 OF 57 REGISTRY COPYRIGHT 1995 ACS  
RN 110078-47-2 REGISTRY  
CN 1,4,8,11-Tetraazacyclotetradecane, 1,1'-[1,4-phenylenebis(methylene)]bis[4,8,11-tris[(4-methylphenyl)sulfonyl]- (9CI) (CA INDEX NAME)  
FS 3D CONCORD  
MF C70 H90 N8 O12 S6  
SR CA  
LC STN Files: CA, CJACS

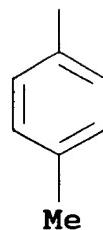
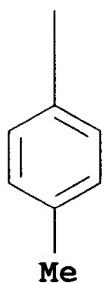
PAGE 1-A



PAGE 1-B



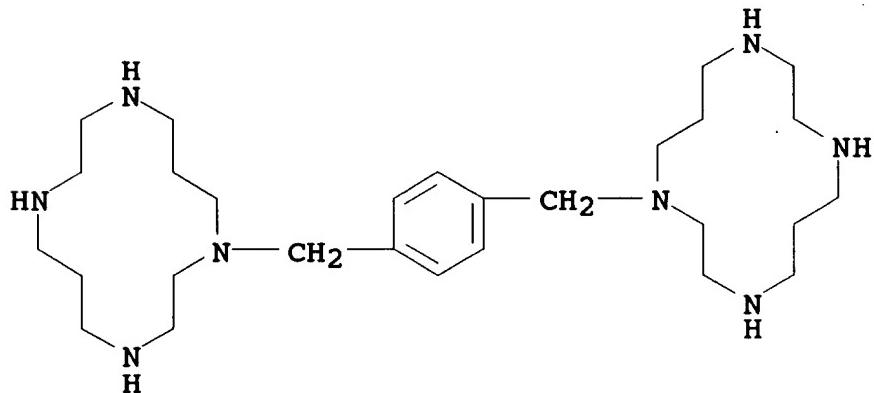
PAGE 2-A



## 1 REFERENCES IN FILE CA (1967 TO DATE)

REFERENCE 1: 107:167695

L46 ANSWER 53 OF 57 REGISTRY COPYRIGHT 1995 ACS  
 RN 110078-46-1 REGISTRY  
 CN 1,4,8,11-Tetraazacyclotetradecane, 1,1'-[1,4-phenylenebis(methylene)]bis- (9CI) (CA INDEX NAME)  
 FS 3D CONCORD  
 MF C28 H54 N8  
 CI COM  
 SR CA  
 LC STN Files: BEILSTEIN\*, CA, CJACS, USPATFULL  
 (\*File contains numerically searchable property data)



## 4 REFERENCES IN FILE CA (1967 TO DATE)

2 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA

REFERENCE 1: P 120:30786

REFERENCE 2: 118:204007

REFERENCE 3: P 114:207294

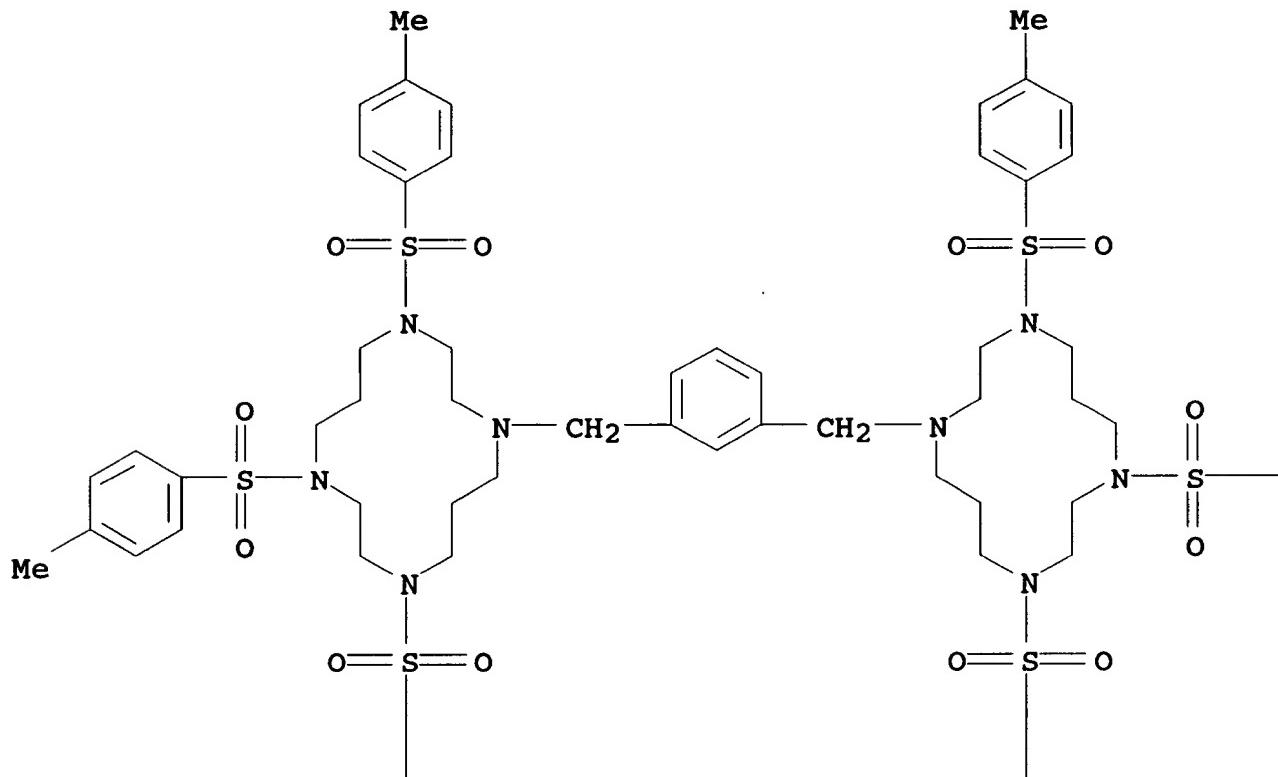
REFERENCE 4: 114:207229

REFERENCE 5: 107:167695

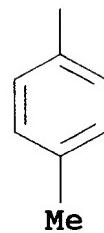
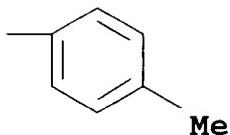
L46 ANSWER 54 OF 57 REGISTRY COPYRIGHT 1995 ACS

RN 110078-45-0 REGISTRY  
CN 1,4,8,11-Tetraazacyclotetradecane, 1,1'-[1,3-  
phenylenebis(methylene)]bis[4,8,11-tris[(4-methylphenyl)sulfonyl]-  
(9CI) (CA INDEX NAME)  
FS 3D CONCORD  
MF C70 H90 N8 O12 S6  
SR CA  
LC STN Files: CA, CJACS

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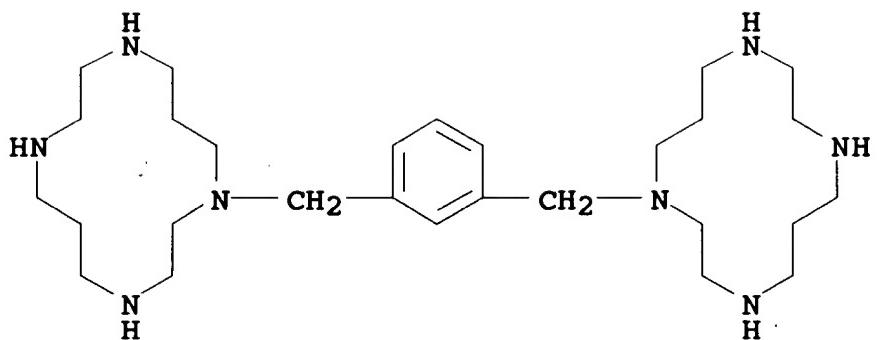


PAGE 2-A

## 1 REFERENCES IN FILE CA (1967 TO DATE)

REFERENCE 1: 107:167695

L46 ANSWER 55 OF 57 REGISTRY COPYRIGHT 1995 ACS  
RN 110078-44-9 REGISTRY  
CN 1,4,8,11-Tetraazacyclotetradecane, 1,1'-[1,3-phenylenebis(methylene)]bis- (9CI) (CA INDEX NAME)  
FS 3D CONCORD  
MF C28 H54 N8  
SR CA  
LC STN Files: BEILSTEIN\*, CA, CHEMINFORMRX, CJACS, TOXLIT, USPATFULL  
(\*File contains numerically searchable property data)



## 5 REFERENCES IN FILE CA (1967 TO DATE)

REFERENCE 1: 120:289504

REFERENCE 2: P 120:30786

REFERENCE 3: P 114:207294

REFERENCE 4: 114:207229

REFERENCE 5: 107:167695

L46 ANSWER 56 OF 57 REGISTRY COPYRIGHT 1995 ACS

RN 105390-46-3 REGISTRY

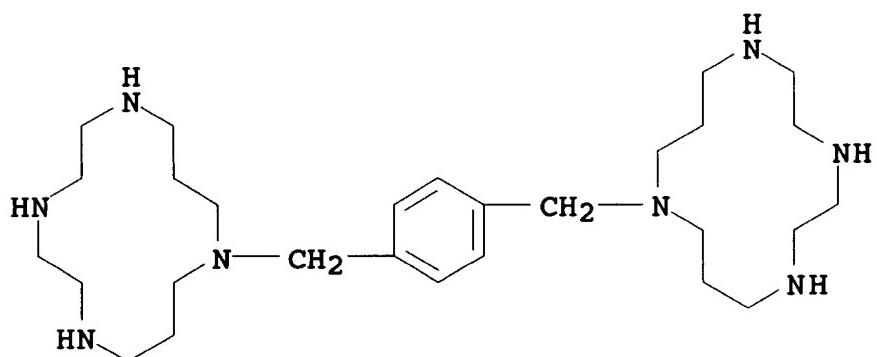
CN 1,4,7,11-Tetraazacyclotetradecane, 11,11'-(1,4-phenylenebis(methylene))bis-, octahydrochloride (9CI) (CA INDEX NAME)

MF C28 H54 N8 . 8 Cl H

SR CA

LC STN Files: CA

CRN (151190-99-7)



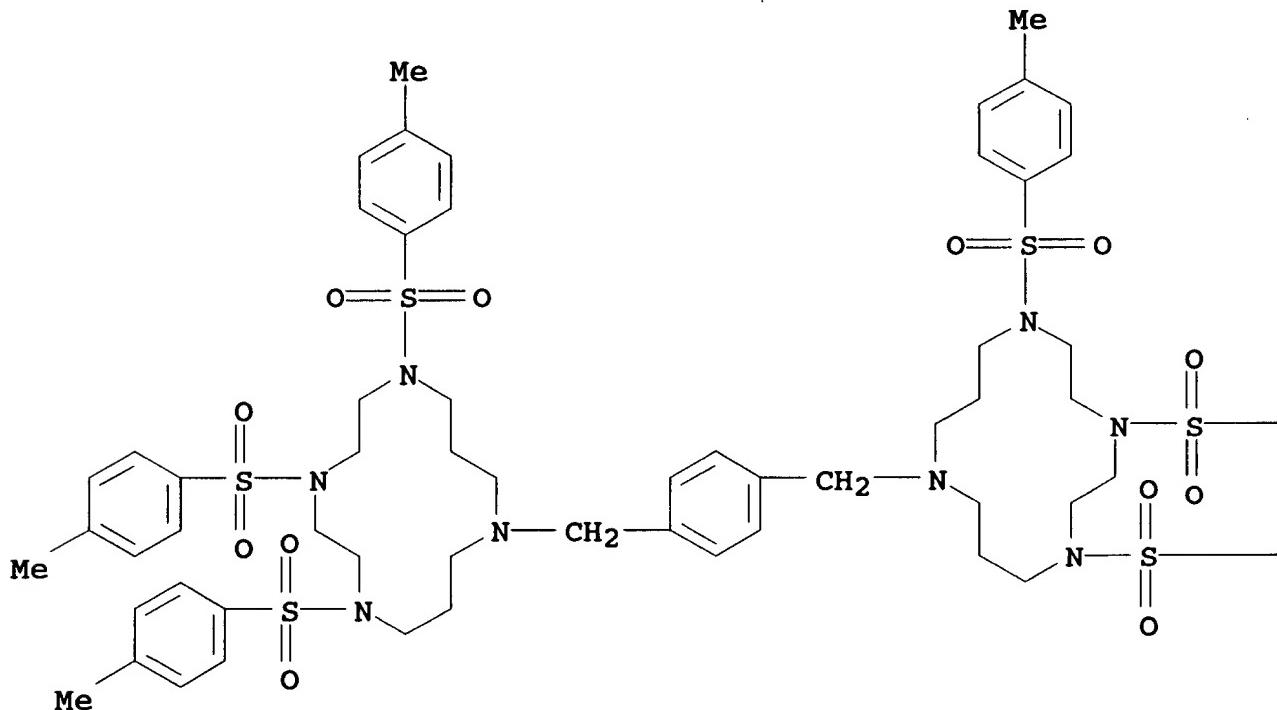
● 8 HCl

## 1 REFERENCES IN FILE CA (1967 TO DATE)

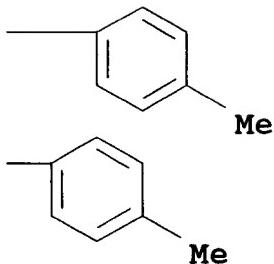
REFERENCE 1: 106:26833

L46 ANSWER 57 OF 57 REGISTRY COPYRIGHT 1995 ACS  
RN 105355-16-6 REGISTRY  
CN 1,4,7,11-Tetraazacyclotetradecane, 11,11'-(1,4-phenylenebis(methylene))bis[1,4,7-tris[(4-methylphenyl)sulfonyl]- (9CI) (CA INDEX NAME)  
FS 3D CONCORD  
MF C70 H90 N8 O12 S6  
SR CA  
LC STN Files: CA

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## 2 REFERENCES IN FILE CA (1967 TO DATE)

REFERENCE 1: P 120:30786

REFERENCE 2: 106:26833

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L47 10 L46

=&gt; d 1-10 bib abs hitrn

L47 ANSWER 1 OF 10 CA COPYRIGHT 1995 ACS

AN 121:225706 CA

TI Synthetic Bis-Metal Ion Receptors for Bis-Imidazole "Protein Analogs"

AU Mallik, Sanku; Johnson, Robert D.; Arnold, Frances H.

CS Division of Chemistry and Chemical Engineering 210-41, California Institute of Technology, Pasadena, CA, 91125, USA

SO J. Am. Chem. Soc. (1994), 116(20), 8902-11

DT CODEN: JACSAT; ISSN: 0002-7863  
LA Journal  
LA English  
OS CJACS-IMAGE; CJACS

AB The authors are investigating an approach to protein recognition that is based on matching a pattern of metal ions in a synthetic receptor to a complementary pattern of metal-coordinating functional groups (histidine) on a protein's surface. In this model study, target "protein analogs" were constructed by linking two imidazoles via org. spacers of varying lengths. By computer modeling the individual targets and receptors, bis-Hg<sup>2+</sup> receptors were designed to position two metal ions to match the available nitrogen ligands of their target bis-imidazoles. While <sup>1</sup>H NMR studies in DMSO-d<sub>6</sub> show that the receptors can bind 2 equiv of 1-benzylimidazole (K<sub>1</sub> .apprx. 104 M<sup>-1</sup>), a bis-imidazole is bound in a 1:1 complex with assocn. consts. as high as 3.times.106 M<sup>-1</sup>. Bis-metal ion receptors are indeed selective for their target bis-imidazoles in competitive binding expts., preferring the target over others that are both longer and shorter by .apprx.4 .ANG. (max. selectivity = 11.5). A max. selectivity of 140 was obsd. for the competition between a target bis-imidazole and 1-benzylimidazole. Increasing the available coordination sites on the metal ion significantly reduces selectivity, presumably by allowing the receptor to take on multiple bound conformations. Attempts to improve binding selectivity by restricting the receptors' conformational mobility reduced selectivity, primarily by introducing unanticipated unfavorable interactions with the target bis-imidazoles.

IT 147025-65-8P 147025-66-9P 158200-25-0P

158200-26-1P

(synthetic bis-metal ion receptors for bis-imidazole protein analogs)

L47 ANSWER 2 OF 10 CA COPYRIGHT 1995 ACS

AN 120:289504 CA

TI Highly potent and selective inhibition of human immunodeficiency virus by the bicyclam derivative JM3100

AU De Clercq, Erik; Yamamoto, Naohiko; Pauwels, Rudi; Balzarini, Jan; Witvrouw, Myriam; De Vreese, Karen; Debyser, Zeger; Rosenwirth, Brigitte; Peichl, Peter; et al.

CS Rega Inst. Med. Res., Kathol. Univ. Leuven, Louvain, B-3000, Belg.

SO Antimicrob. Agents Chemother. (1994), 38(4), 668-74

CODEN: AMACCQ; ISSN: 0066-4804

DT Journal

LA English

AB Bicyclams, in which the cyclam (1,4,8,11-tetraazacyclotetradecane) moieties are tethered via an aliph. bridge (i.e., propylene, as in JM2763) are potent and selective inhibitors of human immunodeficiency virus type 1 (HIV-1) and type-2 (HIV-2) (E. De Clercq, N. Yamamoto, R. Pauwels, M. Baba, D. Schols, H. Nakashima, J. Balzarini, Z. Debyser, B. A., Murrer, D. Schwartz, D. Thornton, G. Bridger, S. Fricker, G. Henson, M. Abrams, and D. Picker, Proc. Natl. Acad. Sci. USA 89:5286-5290, 1992). The authors have now found that the bicyclam JM3100, in which the cyclam moieties are tethered by an arom. bridge [i.e., phenylenebis(methylene)], inhibits the replication of various HIV-1 and HIV-2 strains in various cell lines at a 50% effective concn. (EC<sub>50</sub>) of 1 to 10 ng/mL, which is about 100-fold lower than the concn. required for

JM2763 to inhibit HIV replication and at least 100,000-fold lower than the concn. required for JM2763 to inhibit HIV replication and at least 100,000-fold lower than the cytotoxic concn. (>500 .mu.g/mL). In primary T4 lymphocytes or primary monocytes, JM3100 proved inhibitory to HIV-1 (IIIB) and several clin. HIV-1 isolated at an EC50 of less than 1 ng/mL. On the basis of time-of-addn. expts., JM3100 appeared to interact with a viral uncoating event, and this was further corroborated by an uncoating assay in which RNase sensitivity of [5-3H]uridine-labeled virions was monitored. In addn., but possibly mechanistically related, JM3100 blocks formation of infectious particles. JM3100 was also found to interfere directly with virus-induced syncytium formation, albeit at a higher concn. (1 to 2 .mu.g/mL) than that required for inhibition of viral replication. Following s.c. injection of 10 mg of JM3100 per kg of body wt. to rabbits, anti-HIV activity was detected in serum corresponding to serum drug levels exceeding for at least 6 h by >100-fold the EC50 required to inhibit HIV replication in vitro. When combined with either 3'-azido-2',3'-dideoxythymidine or 2',3'-dideoxyinosine, JM3100 achieved a additive inhibition of HIV replication, and when repeatedly subcultivated in the presence of JM3100, the virus remained insensitive to the compd. for at least 30 passages (120 days) in cell culture.

IT 155148-31-5

(HIV virus inhibition by, mechanism of, structure in relation to, in human cells)

IT 110078-44-9 151191-06-9 151191-09-2

155148-32-6

(HIV virus inhibition by, structure in relation to, in human cells)

L47 ANSWER 3 OF 10 CA COPYRIGHT 1995 ACS

AN 120:44414 CA

TI Functional group convergency in a binuclear dephosphorylation reagent

AU Vance, David H.; Czarnik, Anthony W.

CS Dep. Chem., Ohio State Univ., Columbus, OH, 43210, USA

SO J. Am. Chem. Soc. (1993), 115(25), 12165-6

CODEN: JACSAT; ISSN: 0002-7863

DT Journal

LA English

OS CJACS-IMAGE; CJACS

GI

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

AB Phosphomonoesters experience rapid hydrolysis in the presence of 2 equiv of Co(III) complexes bearing substitutable cis-coordination sites. A binuclear Co(III) complex was synthesized possessing a phosphate-sized pocket, but rigidly so as to avoid .mu.-oxo dimer formation. X-ray anal. of the carbonato form I confirms the cofacial orientation of the metal centers, and <sup>31</sup>P NMR of the phosphate complex II suggests triscoordination of phosphate to Co(III). The binuclear complex at 1 mM affects the dephosphorylation of p-nitrophenyl phosphate 10-times faster than do

either the mononuclear Co(III)-cyclen or Co(III)-trpn complexes at 2 mM.

IT 151987-13-2P

(prep. and crystal structure and aquation of)

IT 151697-44-8P

(prep. and reaction of, with carbonatocobaltate)

IT 151956-64-8P

(prep. and reaction with phosphate and catalysis by, of hydrolysis of phosphate esters)

L47 ANSWER 4 OF 10 CA COPYRIGHT 1995 ACS

AN 120:30786 CA

TI Linked heterocyclic polyamines with activity against HIV

IN Bridger, Gary James; Padmanabhan, Sreenivasan; Skerlj, Renato Tony; Thornton, David Michael

PA Johnson Matthey P.L.C., UK

SO PCT Int. Appl., 66 pp.

CODEN: PIXXD2

PI WO 9312096 A1 930624

DS W: AU, CA, CS, FI, HU, JP, KR, NO, NZ, PL, RU, US

RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE

AI WO 92-GB2334 921216

PRAI GB 91-26677 911216

DT Patent

LA English

OS MARPAT 120:30786

AB The title compds. ZRAR1Y [A = arom. or heteroarom. moiety; R, R1 = (un)substituted alk. chain or heteroatom-contg. chain; Y, Z = cyclic polyamine moieties having 9-32 ring members and 3-8 N atoms in the ring spaced by .gtoreq.2 C atoms from each other] or their acid addn. salts or metal complexes are prep'd. and demonstrated viricidal activity against HIV-1 and HIV-2. Thus, 1,1'-(1,4-phenylenebis(methylene)]bis-1,4,8,11-tetraazacyclotetradecane was prep'd. and demonstrated 50% inhibitory concn. against HIV-1 of 0.006 .mu.g/mL and 50% inhibitory concn. against HIV-2 of <0.01 .mu.g/mL in an assay employing infected MT-4 cells.

IT 151191-32-1 151191-33-2 151191-34-3

(HIV viricidal activity of)

IT 110078-44-9P 110078-46-1DP, copper and zinc complexes 151190-72-6P 151190-73-7P

151190-74-8P 151190-75-9P 151190-76-0P

151190-87-3P 151190-93-1P 151190-94-2P

151190-97-5P 151190-98-6P 151190-99-7P

151191-02-5P 151191-03-6P 151191-05-8P

151191-06-9P 151191-08-1P 151191-09-2P

151191-17-2P 151191-18-3P 151191-20-7P

151191-21-8P 151191-26-3P 151191-27-4P

151191-28-5P 151191-29-6P 151191-30-9P

151191-31-0P

(prep. and HIV viricidal activity of)

IT 105355-16-6P 151190-70-4P 151190-71-5P

151190-86-2P 151190-92-0P 151191-01-4P

151191-04-7P 151191-07-0P 151191-16-1P

151191-19-4P

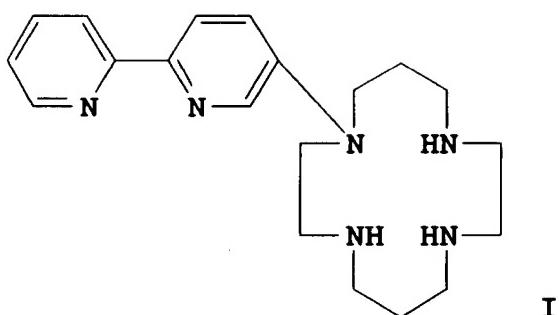
(prep. and reaction of, in prepn. of heterocyclic HIV viricidal agents)

IT 110078-46-1

(reaction of, in prepn. of heterocyclic HIV viricidal agents)

- L47 ANSWER 5 OF 10 CA COPYRIGHT 1995 ACS  
 AN 118:204007 CA  
 TI Selective recognition of bis-imidazoles by complementary bis-metal ion complexes  
 AU Mallik, Sanku; Johnson, Robert D.; Arnold, Frances H.  
 CS Div. Chem. Eng., California Inst. Technol., Pasadena, CA, 91125, USA  
 SO J. Am. Chem. Soc. (1993), 115(6), 2518-20  
 CODEN: JACSAT; ISSN: 0002-7863  
 DT Journal  
 LA English  
 OS CJACS-IMAGE; CJACS
- AB Metal ion complexes capable of selective recognition are made by matching the spatial distribution of metal ions in the complex to the spacing between coordinating ligands on the target mol. Two ligands (L), 1,4-di[(1',4',8',11'-tetraazacyclotetradecan-1'-yl)methylene]benzene (L1) and 2,6-di[(1',4',8',11'-tetraazacyclotetradecan-1'-yl)methylene]naphthalene (L2), were synthesized. The corresponding [Hg<sub>2</sub>(H<sub>2</sub>O)<sub>2</sub>]ClO<sub>4</sub> (3) were designed to bind a bis-imidazole target mol., 4,4'-di(imidazol-1-yl)methylenebiphenyl (2), preferentially over the closely related bis-imidazole, 1,4-di(imidazol-1-yl)xylene (1). From <sup>1</sup>H NMR chem. shifts in titrn. expts. 3 (L = L1) forms a cyclic complex with 2, but not with 1 in DMSO-d<sub>6</sub>. Receptor 3 (L = L1) exhibits a selectivity of 10 in binding 2 over 1; the selectivity is increased to 14 with 3 (L = L2). This model system demonstrates that receptor complexes contg. properly-positioned metal ions can selectively bind target mols. with a complementary spatial distribution of metal-coordinating ligands. Metal ion complexes such as these may have applications as synthetic receptors for biol. mols. such as proteins that are characterized by unique pattern of surface coordinating ligands.
- IT 110078-46-1DP, mercury dinuclear complexes with imidazole derivs. 147025-65-8DP, mercury dinuclear complexes with imidazole derivs.  
 (formation and binding selectivities of)
- IT 147025-66-9P  
 (formation and deprotection of)
- IT 147025-65-8P  
 (prepn. and reaction of, with mercury perchlorate)
- L47 ANSWER 6 OF 10 CA COPYRIGHT 1995 ACS  
 AN 117:82274 CA  
 TI Synthesis and coordination chemistry of 1-(2',2''-bipyridyl-5'-yl-methyl)-1,4,8,11-tetraazacyclotetradecane L1. Quenching of fluorescence from [Ru(bipy)<sub>2</sub>(L1)]<sup>2+</sup> by coordination of Ni<sup>II</sup> or Cu<sup>II</sup> in the cyclam cavity (bipy = 2,2'-bipyridine; cyclam = 1,4,8,11-tetraazacyclotetradecane)  
 AU Rawle, Simon C.; Moore, Peter; Alcock, Nathaniel W.  
 CS Dep. Chem., Univ. Warwick, Coventry, CV4 7AL, UK  
 SO J. Chem. Soc., Chem. Commun. (1992), (9), 684-7  
 CODEN: JCCCAT; ISSN: 0022-4936  
 DT Journal  
 LA English  
 OS CJRSC

GI

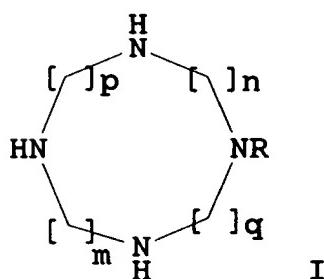


AB A novel bipy deriv. (I) of cyclam, designed for controlled and systematic polynuclear metal complex formation, is reported. Fluorescence quenching of the  $[\text{Ru}(\text{bipy})_2]^{2+}$  core of  $[(\text{bipy})_2\text{RuL}]^{2+}$  ( $\text{L} = \text{I}$ ) upon coordination of CuII at the cyclam cavity is demonstrated. The crystal structure of  $[\text{CuL}](\text{ClO}_4)_2 \cdot \text{MeNO}_2$  was detd.

IT 142079-95-6P

(prepn. of)

L47 ANSWER 7 OF 10 CA COPYRIGHT 1995 ACS  
 AN 114:207294 CA  
 TI Preparation of mono-N-substituted cyclic tetramines  
 IN Handel, Henri; Yaouanc, Jean Jacques; Filali Zegzouti, Ayoub;  
 Malouala, Denis; Des Abbayes, Herve; Clement, Jean Claude; Bernard,  
 Helene; Le Gall, Guenaelle  
 PA Centre National de la Recherche Scientifique, Fr.  
 SO Eur. Pat. Appl., 20 pp. U.S. 5,047,527 X  
 CODEN: EPXXDW  
 PI EP 389359 A1 900926  
 DS R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE  
 AI EP 90-400762 900320  
 PRAI FR 89-3600 890320  
 DT Patent  
 LA French  
 OS MARPAT 114:207294  
 GI



AB The title compds. [I; R = (un)satd. org. radical; m-q = 2, 3; m = n = 2 and p = 1 = 3; m = 2 and n-q = 3; n = 2 and m = p = q = 3; m = n

= 3 and p = q = 4] were prep'd. by substitution of I (R = H) in which 3 N-atoms are coordinated to a central group, e.g., M(CO)<sub>3</sub> (M = Cr, Mo, W). Thus, cyclam was refluxed 2-3 h with Cr(CO)<sub>6</sub> in deaerated Bu<sub>2</sub>O and the product heated 2 h at 100.degree. with PhCH<sub>2</sub>Br in DMF contg. Na<sub>2</sub>CO<sub>3</sub> to give I (R = PhCH<sub>2</sub>; m = n = 2, q = 3).

IT 110078-44-9P 110078-46-1P 133563-60-7P  
(prepn. of, method for)

L47 ANSWER 8 OF 10 CA COPYRIGHT 1995 ACS

AN 114:207229 CA

TI Mono N-functionalization of cyclic and linear tetraamines via their tridentate tricarbonylchromium complexes

AU Yaouanc, Jean Jacques; Le Bris, Nathalie; Le Gall, Guenaelle; Clement, Jean Claude; Handel, Henri; Des Abbayes, Herve

CS Fac. Sci. Tech., Brest, 29287, Fr.

SO J. Chem. Soc., Chem. Commun. (1991), (4), 206-7

CODEN: JCCCAT; ISSN: 0022-4936

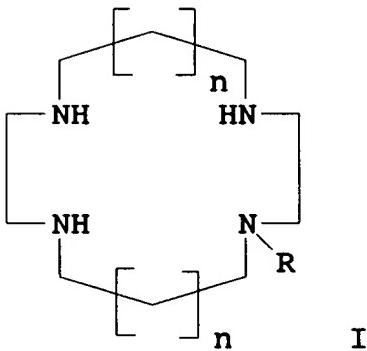
DT Journal

LA English

OS CJRSC

GI

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AB Cyclic tetraamines I (R = H, n = 0, 1) and H<sub>2</sub>N(CH<sub>2</sub>)<sub>n</sub>NHCH<sub>2</sub>CH<sub>2</sub>NH(CH<sub>2</sub>)<sub>n</sub>NH<sub>2</sub> (n = 2, 3) were selectively monoalkylated in high yield at the uncomplexed N of a Cr(CO)<sub>3</sub> tridentate complex. Thus, I (R = H) upon treatment with Cr(CO)<sub>6</sub> in Bu<sub>2</sub>O at 142.degree. gave 85-90% of a tridentate complex, which on treatment with PhCH<sub>2</sub>Br in DMF at 100.degree. followed by decomplexation afforded 85-95% (R = CH<sub>2</sub>Ph).

IT 110078-44-9P 110078-46-1P

(prepn. of, by monoalkylation of tridentate chromium carbonyl complex)

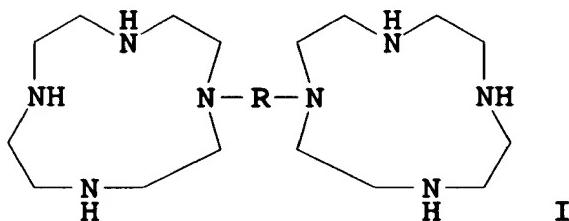
L47 ANSWER 9 OF 10 CA COPYRIGHT 1995 ACS

AN 107:167695 CA

TI Dinickel and dicopper complexes with N,N-linked bis(cyclam) ligands. An ideal system for the investigation of electrostatic effects on the redox behavior of pairs of metal ions

AU Ciampolini, Mario; Fabbrizzi, Luigi; Perotti, Angelo; Poggi, Antonio; Seghi, Barbara; Zanobini, Fabrizio

CS Dip. Chim. Gen., Univ. Pavia, Pavia, 27100, Italy  
 SO Inorg. Chem. (1987), 26(21), 3527-33  
 CODEN: INOCAJ; ISSN: 0020-1669  
 DT Journal ✓  
 LA English  
 OS CJACS  
 GI



AB I ( $R = (CH_2)_2, (CH_2)_3, (CH_2)_4, m\text{-xylyl}, p\text{-xylyl}$ ) were prep'd. by condensation of  $N,N',N''\text{-tritosylcyclam}$  (2 equiv) with an  $XRX$  fragment ( $X = Br$  or  $OTs$ ).  $M_2L4+$  ( $M = Ni, Cu$ ;  $H_4L = I$ ) undergo a 2-electron-oxidn. process, according to 2 reversible 1-electron steps, whose redox potentials are sep'd. by the quantity  $\Delta E$ . The value of  $\Delta E$  is related to the comproportionation (or valence scrambling) equil.  $[MIIIMIIIIL]^{6+} + [MIIMIIL]^{4+} \rightleftharpoons 2[MIIIMIIL]^{5+}$  and results from the combination of a statistical fixed contribution and a term that reflects the electrostatic repulsion between the metal centers of the dinuclear complex. The electrostatic repulsion term decreases when the distance between the metal centers is increased, according to a hyperbolic mode, but does not show any definite dependence upon the macroscopic values of the dielec. const. of the explored media. Moreover, the electrostatic term significantly varies with the stereochem. features of each metal center in its oxidn. state (II or III), which cannot be any longer considered as simple point charges.

IT 110078-45-0P 110078-47-2P  
 (prepn. and detosylation of)  
 IT 110078-44-9P 110078-46-1P  
 (prepn. of)

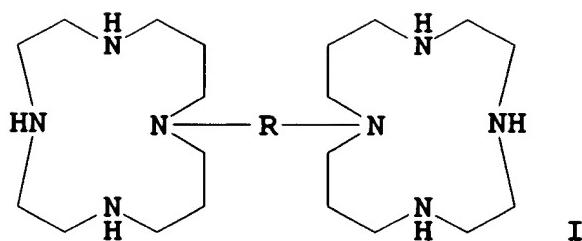
L47 ANSWER 10 OF 10 CA COPYRIGHT 1995 ACS

AN 106:26833 CA

TI Metal complexes with macrocyclic ligands. Part XXII. Synthesis of two bis(tetraaza)macrocycles and study of the structures, electrochemistry, visible and ESR spectra of their binuclear copper(2+) and nickel(2+) complexes

AU Schneider, Rene; Riesen, Andreas; Kaden, Thomas A.  
 CS Inst. Anorg. Chem., Univ. Basel, Basel, CH-4056, Switz.  
 SO Helv. Chim. Acta (1986), 69(1), 53-61  
 CODEN: HCACAV; ISSN: 0018-019X

DT Journal  
 LA English  
 GI



AB I ( $R = p\text{-CH}_2\text{C}_6\text{H}_4\text{CH}_2, \text{CH}_2\text{CH}_2$ ) were prep'd. by 1,4,7-tritosyl-1,4,7,11-tetraazacyclotetradecane as starting compd. and bifunctional alkylating agents. The bis-macrocycles give binuclear complexes with  $\text{Ni}^{2+}$  and  $\text{Cu}^{2+}$ , the properties of which were studied to obtain information about the interaction of the 2 subunits as a function of the distance. The visible spectra of the  $\text{Ni}^{2+}$  and  $\text{Cu}^{2+}$  complexes indicate that both metal ions are in a square-planar geometry as expected from the result of the analogous complexes with 1,4,7,11-tetraazacyclotetradecane. Cyclic voltammetry and differential pulse polarog. of the binuclear  $\text{Ni}^{2+}$  complexes in  $\text{CH}_3\text{CN}$  show a single 2-electron step for I ( $R = \text{CH}_2\text{CH}_2$ ), whereas 2 distinct 1-electron redox processes can be obsd. for I ( $R = p\text{-CH}_2\text{C}_6\text{H}_4\text{CH}_2$ ), indicating that the 2 metal ions interact with each other when the chain length is shorter. Similarly, the EPE studies of frozen solns. of the binuclear  $\text{Cu}^{2+}$  complexes clearly show that a magnetic dipolar interaction between the 2 paramagnetic centers exists, and that the strength of it depends upon the length of the bridge. Finally, from the x-ray structures of the binuclear  $\text{Ni}^{2+}$  complexes with I, 2 rings are kept apart as far as possible; the distances between the two metal ions detd. in the solid correlate well with the observation in soln.

IT 105355-16-6P

(prepn. and deblocking of)

IT 105390-46-3P

(prepn. of)